1,2-Benzenedicarboxylic acid, diheptyl ester

Other names:	Di-n-heptyl phthalate
	Diheptyl phthalate
	Heptyl phthalate
	Phthalic acid, diheptyl ester
	diheptyl 1,2-benzenedicarboxylate
	diheptyl benzene-1,2-dicarboxylate
Inchi:	InChI=1S/C22H34O4/c1-3-5-7-9-13-17-25-21(23)19-15-11-12-16-20(19)22(24)26-18-14-
InchiKey:	JQCXWCOOWVGKMT-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCC
Mol. weight [g/mol]:	362.50
CAS:	3648-21-3

Physical Properties

Property code	Value	Unit	Source
gf	-230.70	kJ/mol	Joback Method
hf	-761.95	kJ/mol	Joback Method
hfus	51.96	kJ/mol	Joback Method
hvap	85.82	kJ/mol	Joback Method
log10ws	-8.56		Aqueous Solubility Prediction Method
logp	5.941		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1240.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method
rinpol	2497.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2453.00		NIST Webbook
rinpol	2497.00		NIST Webbook
rinpol	2494.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2500.00		NIST Webbook
rinpol	416.50		NIST Webbook
rinpol	416.50		NIST Webbook
rinpol	2494.00		NIST Webbook
rinpol	2500.00		NIST Webbook

rinpol	2472.00		NIST Webbook
rinpol	2497.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	887.00	K	Joback Method
tc	1090.20	K	Joback Method
tf	520.96	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.29	J/mol×K	887.00	Joback Method
cpg	1068.08	J/mol×K	1056.33	Joback Method
cpg	1056.27	J/mol×K	1022.47	Joback Method
cpg	1043.31	J/mol×K	988.60	Joback Method
cpg	1029.18	J/mol×K	954.73	Joback Method
cpg	1013.85	J/mol×K	920.87	Joback Method
cpg	1078.77	J/mol×K	1090.20	Joback Method
dvisc	0.0000413	Pa×s	887.00	Joback Method
dvisc	0.0000534	Pa×s	825.99	Joback Method
dvisc	0.0000721	Pa×s	764.99	Joback Method
dvisc	0.0001024	Pa×s	703.98	Joback Method
dvisc	0.0001556	Pa×s	642.97	Joback Method
dvisc	0.0002579	Pa×s	581.97	Joback Method
dvisc	0.0004813	Pa×s	520.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	487.50 ± 0.50	K	0.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3648213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method:	https://www.doi.org/10.1021/je060068f
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume