

1,3-Benzenedicarboxylic acid, diheptyl ester

Inchi:	InChI=1S/C22H34O4/c1-3-5-7-9-11-16-25-21(23)19-14-13-15-20(18-19)22(24)26-17-12-
InchiKey:	NRVRCDIOAWDMJQ-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCC)c1
Mol. weight [g/mol]:	362.50

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	-6.98		Crippen Method
logp	5.941		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2605.00		NIST Webbook
rinpol	2605.00		NIST Webbook
rinpol	2608.00		NIST Webbook
rinpol	2605.00		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/molxK	887.00	Joback Method
cpg	1013.85	J/molxK	920.87	Joback Method
cpg	1029.18	J/molxK	954.73	Joback Method
cpg	1043.31	J/molxK	988.60	Joback Method
cpg	1056.27	J/molxK	1022.47	Joback Method
cpg	1068.08	J/molxK	1056.33	Joback Method

cpg	1078.77	J/molxK	1090.20	Joback Method
dvisc	0.0004813	Paxs	520.96	Joback Method
dvisc	0.0002579	Paxs	581.97	Joback Method
dvisc	0.0001556	Paxs	642.97	Joback Method
dvisc	0.0001024	Paxs	703.98	Joback Method
dvisc	0.0000721	Paxs	764.99	Joback Method
dvisc	0.0000534	Paxs	825.99	Joback Method
dvisc	0.0000413	Paxs	887.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R15098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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