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/mol×K	887.00	Joback Method
cpg	1013.85	J/mol×K	920.87	Joback Method
cpg	1029.18	J/mol×K	954.73	Joback Method
cpg	1043.31	J/mol×K	988.60	Joback Method
cpg	1056.27	J/mol×K	1022.47	Joback Method
cpg	1068.08	J/mol×K	1056.33	Joback Method

cpg	1078.77	J/mol×K	1090.20	Joback Method
dvisc	0.0004813	Pa×s	520.96	Joback Method
dvisc	0.0002579	Pa×s	581.97	Joback Method
dvisc	0.0001556	Pa×s	642.97	Joback Method
dvisc	0.0001024	Pa×s	703.98	Joback Method
dvisc	0.0000721	Pa×s	764.99	Joback Method
dvisc	0.0000534	Pa×s	825.99	Joback Method
dvisc	0.0000413	Pa×s	887.00	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
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/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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