Isophthalic acid, neopentyl tetradecyl ester

Inchi: InChI=1S/C27H44O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-20-30-25(28)23-18-17-19-24(2
InchiKey: OHJVCUNAJOREOY-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-185.76	kJ/mol	Joback Method
hf	-873.90	kJ/mol	Joback Method
hfus	57.50	kJ/mol	Joback Method
hvap	95.65	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.747		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	873.77	kPa	Joback Method
rinpol	3149.00		NIST Webbook
rinpol	3149.00		NIST Webbook
tb	998.17	K	Joback Method
tc	1222.43	K	Joback Method
tf	579.73	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.32	J/mol×K	998.17	Joback Method
cpg	1381.47	J/mol×K	1185.06	Joback Method
cpg	1369.08	J/mol×K	1147.68	Joback Method
cpg	1355.45	J/mol×K	1110.30	Joback Method
cpg	1340.50	J/mol×K	1072.92	Joback Method
cpg	1324.15	J/mol×K	1035.55	Joback Method
cpg	1392.70	J/mol×K	1222.43	Joback Method
dvisc	0.0000148	Pa×s	998.17	Joback Method

dvisc	0.0000197	Pa×s	928.43	Joback Method
dvisc	0.0000274	Pa×s	858.69	Joback Method
dvisc	0.0000406	Pa×s	788.95	Joback Method
dvisc	0.0000649	Pa×s	719.21	Joback Method
dvisc	0.0001146	Pa×s	649.47	Joback Method
dvisc	0.0002323	Pa×s	579.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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