

Isophthalic acid, hexadecyl 3-methylbutyl ester

Inchi:	InChI=1S/C29H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-32-28(30)26-19-18-20
InchiKey:	JZIQLFUKDKDOX-UHFFFAOYSA-N
Formula:	C29H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)c1
Mol. weight [g/mol]:	460.69

Physical Properties

Property code	Value	Unit	Source
gf	-174.20	kJ/mol	Joback Method
hf	-911.71	kJ/mol	Joback Method
hfus	66.57	kJ/mol	Joback Method
hvap	101.01	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.528		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	777.64	kPa	Joback Method
rinpol	3351.00		NIST Webbook
tb	1046.72	K	Joback Method
tc	1288.88	K	Joback Method
tf	584.85	K	Joback Method
vc	1.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.30	J/molxK	1046.72	Joback Method
cpg	1451.71	J/molxK	1087.08	Joback Method
cpg	1468.21	J/molxK	1127.44	Joback Method
cpg	1482.86	J/molxK	1167.80	Joback Method
cpg	1495.77	J/molxK	1208.16	Joback Method
cpg	1507.00	J/molxK	1248.52	Joback Method
cpg	1516.63	J/molxK	1288.88	Joback Method
dvisc	0.0002283	Paxs	584.85	Joback Method
dvisc	0.0001073	Paxs	661.83	Joback Method

dvisc	0.0000590	Paxs	738.81	Joback Method
dvisc	0.0000363	Paxs	815.78	Joback Method
dvisc	0.0000243	Paxs	892.76	Joback Method
dvisc	0.0000173	Paxs	969.74	Joback Method
dvisc	0.0000130	Paxs	1046.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356471&Units=SI

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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