

Isophthalic acid, hexadecyl neopentyl ester

Inchi:	InChI=1S/C29H48O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-32-27(30)25-20-19-2
InchiKey:	BFRHELRLRXTIW-UHFFFAOYSA-N
Formula:	C29H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]:	460.69

Physical Properties

Property code	Value	Unit	Source
gf	-168.92	kJ/mol	Joback Method
hf	-915.18	kJ/mol	Joback Method
hfus	62.68	kJ/mol	Joback Method
hvap	100.10	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.528		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	782.43	kPa	Joback Method
rinpol	3356.00		NIST Webbook
rinpol	3356.00		NIST Webbook
tb	1043.93	K	Joback Method
tc	1282.64	K	Joback Method
tf	602.27	K	Joback Method
vc	1.589	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.98	J/molxK	1043.93	Joback Method
cpg	1451.55	J/molxK	1083.72	Joback Method
cpg	1468.47	J/molxK	1123.50	Joback Method
cpg	1483.84	J/molxK	1163.29	Joback Method
cpg	1497.76	J/molxK	1203.07	Joback Method
cpg	1510.33	J/molxK	1242.86	Joback Method
cpg	1521.67	J/molxK	1282.64	Joback Method
dvisc	0.0001776	Paxs	602.27	Joback Method

dvisc	0.0000861	Paxs	675.88	Joback Method
dvisc	0.0000482	Paxs	749.49	Joback Method
dvisc	0.0000299	Paxs	823.10	Joback Method
dvisc	0.0000201	Paxs	896.71	Joback Method
dvisc	0.0000143	Paxs	970.32	Joback Method
dvisc	0.0000107	Paxs	1043.93	Joback Method

Sources

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=U343873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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