

Isophthalic acid, neopentyl pentadecyl ester

Inchi:	InChI=1S/C28H46O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21-31-26(29)24-19-18-20-2
InchiKey:	JTMUNRTPBEAFH-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]:	446.66

Physical Properties

Property code	Value	Unit	Source
gf	-177.34	kJ/mol	Joback Method
hf	-894.54	kJ/mol	Joback Method
hfus	60.09	kJ/mol	Joback Method
hvap	97.88	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.137		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	826.21	kPa	Joback Method
rinpol	3251.00		NIST Webbook
rinpol	3251.00		NIST Webbook
tb	1021.05	K	Joback Method
tc	1251.94	K	Joback Method
tf	591.00	K	Joback Method
vc	1.532	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.45	J/molxK	1021.05	Joback Method
cpg	1387.63	J/molxK	1059.53	Joback Method
cpg	1404.25	J/molxK	1098.01	Joback Method
cpg	1419.40	J/molxK	1136.49	Joback Method
cpg	1433.16	J/molxK	1174.98	Joback Method
cpg	1445.64	J/molxK	1213.46	Joback Method
cpg	1456.91	J/molxK	1251.94	Joback Method
dvisc	0.0002033	Paxs	591.00	Joback Method

dvisc	0.0000995	Paxs	662.67	Joback Method
dvisc	0.0000560	Paxs	734.35	Joback Method
dvisc	0.0000349	Paxs	806.02	Joback Method
dvisc	0.0000235	Paxs	877.70	Joback Method
dvisc	0.0000168	Paxs	949.38	Joback Method
dvisc	0.0000126	Paxs	1021.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343872&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
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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