

Isophthalic acid, neopentyl undecyl ester

Inchi:	InChI=1S/C24H38O4/c1-5-6-7-8-9-10-11-12-13-17-27-22(25)20-15-14-16-21(18-20)23(2
InchiKey:	GVNDVMVHZIGBMH-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-211.02	kJ/mol	Joback Method
hf	-811.98	kJ/mol	Joback Method
hfus	49.73	kJ/mol	Joback Method
hvap	88.97	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.577		Crippen Method
mvol	340.140	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook
tb	929.53	K	Joback Method
tc	1140.30	K	Joback Method
tf	545.92	K	Joback Method
vc	1.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.60	J/molxK	929.53	Joback Method
cpg	1136.63	J/molxK	964.66	Joback Method
cpg	1152.36	J/molxK	999.79	Joback Method
cpg	1166.86	J/molxK	1034.91	Joback Method
cpg	1180.17	J/molxK	1070.04	Joback Method
cpg	1192.37	J/molxK	1105.17	Joback Method
cpg	1203.50	J/molxK	1140.30	Joback Method
dvisc	0.0003412	Paxs	545.92	Joback Method

dvisc	0.0001732	Paxs	609.86	Joback Method
dvisc	0.0001000	Paxs	673.79	Joback Method
dvisc	0.0000635	Paxs	737.72	Joback Method
dvisc	0.0000434	Paxs	801.66	Joback Method
dvisc	0.0000313	Paxs	865.59	Joback Method
dvisc	0.0000237	Paxs	929.53	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=U343869&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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