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: CCCCCCCCCCCOC(=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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001732	Pa×s	609.86	Joback Method
dvisc	0.0001000	Pa×s	673.79	Joback Method
dvisc	0.0000635	Pa×s	737.72	Joback Method
dvisc	0.0000434	Pa×s	801.66	Joback Method
dvisc	0.0000313	Pa×s	865.59	Joback Method
dvisc	0.0000237	Pa×s	929.53	Joback Method

Sources

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
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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