Isophthalic acid, dodecyl neopentyl ester

Inchi: InChI=1S/C25H40O4/c1-5-6-7-8-9-10-11-12-13-14-18-28-23(26)21-16-15-17-22(19-21)2
InchiKey: XAONYSPQOOPDLP-UHFFFAOYSA-N
Formula: C25H40O4
SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-202.60	kJ/mol	Joback Method
hf	-832.62	kJ/mol	Joback Method
hfus	52.32	kJ/mol	Joback Method
hvap	91.20	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	6.967		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	982.08	kPa	Joback Method
rinpol	2932.00		NIST Webbook
rinpol	2932.00		NIST Webbook
tb	952.41	K	Joback Method
tc	1166.68	K	Joback Method
tf	557.19	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.34	J/mol×K	952.41	Joback Method
cpg	1198.60	J/mol×K	988.12	Joback Method
cpg	1214.52	J/mol×K	1023.83	Joback Method
cpg	1229.15	J/mol×K	1059.55	Joback Method
cpg	1242.56	J/mol×K	1095.26	Joback Method
cpg	1254.81	J/mol×K	1130.97	Joback Method
cpg	1265.98	J/mol×K	1166.68	Joback Method
dvisc	0.0003009	Pa×s	557.19	Joback Method

dvisc	0.0001513	Pa×s	623.06	Joback Method
dvisc	0.0000868	Pa×s	688.93	Joback Method
dvisc	0.0000548	Pa×s	754.80	Joback Method
dvisc	0.0000373	Pa×s	820.67	Joback Method
dvisc	0.0000269	Pa×s	886.54	Joback Method
dvisc	0.0000203	Pa×s	952.41	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=U343870&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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