

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:	CCCCCCCCCCCCOC(=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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001513	Paxs	623.06	Joback Method
dvisc	0.0000868	Paxs	688.93	Joback Method
dvisc	0.0000548	Paxs	754.80	Joback Method
dvisc	0.0000373	Paxs	820.67	Joback Method
dvisc	0.0000269	Paxs	886.54	Joback Method
dvisc	0.0000203	Paxs	952.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343870&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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