

Isophthalic acid, 8-chlorooctyl nonyl ester

Inchi:	InChI=1S/C25H39ClO4/c1-2-3-4-5-7-10-13-19-29-24(27)22-16-15-17-23(21-22)25(28)30
InchiKey:	RDDBJPGALIAUSV-UHFFFAOYSA-N
Formula:	C25H39ClO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCl)c1
Mol. weight [g/mol]:	439.03

Physical Properties

Property code	Value	Unit	Source
gf	-217.37	kJ/mol	Joback Method
hf	-839.61	kJ/mol	Joback Method
hfus	63.93	kJ/mol	Joback Method
hvap	96.88	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	7.330		Crippen Method
mvol	366.470	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	3291.00		NIST Webbook
rinpol	3291.00		NIST Webbook
tb	993.07	K	Joback Method
tc	1216.15	K	Joback Method
tf	584.69	K	Joback Method
vc	1.425	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.72	J/molxK	993.07	Joback Method
cpg	1223.86	J/molxK	1030.25	Joback Method
cpg	1238.49	J/molxK	1067.43	Joback Method
cpg	1251.68	J/molxK	1104.61	Joback Method
cpg	1263.48	J/molxK	1141.79	Joback Method
cpg	1273.94	J/molxK	1178.97	Joback Method
cpg	1283.10	J/molxK	1216.15	Joback Method
dvisc	0.0002716	Paxs	584.69	Joback Method

dvisc	0.0001441	Paxs	652.75	Joback Method
dvisc	0.0000862	Paxs	720.82	Joback Method
dvisc	0.0000563	Paxs	788.88	Joback Method
dvisc	0.0000394	Paxs	856.94	Joback Method
dvisc	0.0000290	Paxs	925.01	Joback Method
dvisc	0.0000223	Paxs	993.07	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=U356393&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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