

Isophthalic acid, cyclohexylmethyl dodecyl ester

Inchi:	InChI=1S/C27H42O4/c1-2-3-4-5-6-7-8-9-10-14-20-30-26(28)24-18-15-19-25(21-24)27(29)
InchiKey:	QOZLNVJFHYODSU-UHFFFAOYSA-N
Formula:	C27H42O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]:	430.62

Physical Properties

Property code	Value	Unit	Source
gf	-164.15	kJ/mol	Joback Method
hf	-810.83	kJ/mol	Joback Method
hfus	56.75	kJ/mol	Joback Method
hvap	97.38	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	7.501		Crippen Method
mvol	371.550	ml/mol	McGowan Method
pc	978.40	kPa	Joback Method
rinpol	3396.00		NIST Webbook
rinpol	3396.00		NIST Webbook
tb	1020.95	K	Joback Method
tc	1250.04	K	Joback Method
tf	584.69	K	Joback Method
vc	1.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.74	J/molxK	1020.95	Joback Method
cpg	1317.35	J/molxK	1059.13	Joback Method
cpg	1332.17	J/molxK	1097.31	Joback Method
cpg	1345.24	J/molxK	1135.49	Joback Method
cpg	1356.63	J/molxK	1173.67	Joback Method
cpg	1366.42	J/molxK	1211.86	Joback Method
cpg	1374.66	J/molxK	1250.04	Joback Method
dvisc	0.0002982	Paxs	584.69	Joback Method

dvisc	0.0001482	Paxs	657.40	Joback Method
dvisc	0.0000847	Paxs	730.11	Joback Method
dvisc	0.0000535	Paxs	802.82	Joback Method
dvisc	0.0000365	Paxs	875.53	Joback Method
dvisc	0.0000264	Paxs	948.24	Joback Method
dvisc	0.0000200	Paxs	1020.95	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=U343834&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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