Isophthalic acid, cyclohexylmethyl decyl ester

Inchi: InChI=1S/C25H38O4/c1-2-3-4-5-6-7-8-12-18-28-24(26)22-16-13-17-23(19-22)25(27)29-2
InchiKey: LYQPYCKOQOXKCV-UHFFFAOYSA-N
Formula: C25H38O4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-180.99	kJ/mol	Joback Method
hf	-769.55	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	92.92	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.721		Crippen Method
mcvol	343.370	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rinpol	3186.00		NIST Webbook
rinpol	3186.00		NIST Webbook
tb	975.19	K	Joback Method
tc	1197.03	K	Joback Method
tf	562.15	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.29	J/mol×K	975.19	Joback Method
cpg	1192.94	J/mol×K	1012.16	Joback Method
cpg	1207.94	J/mol×K	1049.14	Joback Method
cpg	1221.31	J/mol×K	1086.11	Joback Method
cpg	1233.13	J/mol×K	1123.09	Joback Method
cpg	1243.43	J/mol×K	1160.06	Joback Method
cpg	1252.27	J/mol×K	1197.03	Joback Method
dvisc	0.0003825	Pa×s	562.15	Joback Method

dvisc	0.0001936	Pa×s	630.99	Joback Method
dvisc	0.0001121	Pa×s	699.83	Joback Method
dvisc	0.0000715	Pa×s	768.67	Joback Method
dvisc	0.0000492	Pa×s	837.51	Joback Method
dvisc	0.0000358	Pa×s	906.35	Joback Method
dvisc	0.0000272	Pa×s	975.19	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=U343832&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