Isophthalic acid, 2-cyclohexylethyl hexyl ester

Inchi: InChI=1S/C22H32O4/c1-2-3-4-8-15-25-21(23)19-12-9-13-20(17-19)22(24)26-16-14-18-1
InchiKey: DKHROGNZAUISSX-UHFFFAOYSA-N
Formula: C22H32O4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCCC2CCCCC2)c1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-206.25	kJ/mol	Joback Method
hf	-707.63	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	86.24	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.551		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2844.00		NIST Webbook
rinpol	2844.00		NIST Webbook
tb	906.55	K	Joback Method
tc	1124.45	K	Joback Method
tf	528.34	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.66	J/mol×K	906.55	Joback Method
cpg	1009.49	J/mol×K	942.87	Joback Method
cpg	1024.79	J/mol×K	979.18	Joback Method
cpg	1038.59	J/mol×K	1015.50	Joback Method
cpg	1050.93	J/mol×K	1051.82	Joback Method
cpg	1061.85	J/mol×K	1088.13	Joback Method
cpg	1071.38	J/mol×K	1124.45	Joback Method
dvisc	0.0005434	Pa×s	528.34	Joback Method

dvisc	0.0002835	Pa×s	591.37	Joback Method
dvisc	0.0001677	Pa×s	654.41	Joback Method
dvisc	0.0001087	Pa×s	717.44	Joback Method
dvisc	0.0000756	Pa×s	780.48	Joback Method
dvisc	0.0000555	Pa×s	843.51	Joback Method
dvisc	0.0000426	Pa×s	906.55	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=U343813&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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