Isophthalic acid, 2-cyclohexylethyl decyl ester

Inchi: InChI=1S/C26H40O4/c1-2-3-4-5-6-7-8-12-19-29-25(27)23-16-13-17-24(21-23)26(28)30-2
InchiKey: IQUCMVGATXHUHB-UHFFFAOYSA-N
Formula: C26H40O4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC2CCCCC2)c1
Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-172.57	kJ/mol	Joback Method
hf	-790.19	kJ/mol	Joback Method
hfus	54.16	kJ/mol	Joback Method
hvap	95.15	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.111		Crippen Method
mcvol	357.460	ml/mol	McGowan Method
pc	1039.91	kPa	Joback Method
rinpol	3279.00		NIST Webbook
rinpol	3279.00		NIST Webbook
tb	998.07	K	Joback Method
tc	1223.03	K	Joback Method
tf	573.42	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.34	J/mol×K	998.07	Joback Method
cpg	1254.97	J/mol×K	1035.56	Joback Method
cpg	1269.87	J/mol×K	1073.06	Joback Method
cpg	1283.09	J/mol×K	1110.55	Joback Method
cpg	1294.70	J/mol×K	1148.05	Joback Method
cpg	1304.76	J/mol×K	1185.54	Joback Method
cpg	1313.31	J/mol×K	1223.03	Joback Method
dvisc	0.0003382	Pa×s	573.42	Joback Method

dvisc	0.0001696	Pa×s	644.20	Joback Method
dvisc	0.0000975	Pa×s	714.97	Joback Method
dvisc	0.0000619	Pa×s	785.75	Joback Method
dvisc	0.0000424	Pa×s	856.52	Joback Method
dvisc	0.0000308	Pa×s	927.29	Joback Method
dvisc	0.0000234	Pa×s	998.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343815&Units=SI
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

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