Isophthalic acid, di(6-ethyloct-3-yl) ester

Inchi: InChI=1S/C28H46O4/c1-7-21(8-2)16-18-25(11-5)31-27(29)23-14-13-15-24(20-23)28(30)
InchiKey: VFWKKILWHHEGHO-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCC(CC)CCC(CC)OC(=O)c1cccc(C(=O)OC(CC)CCC(CC)CC)c1
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-189.94	kJ/mol	Joback Method
hf	-906.91	kJ/mol	Joback Method
hfus	53.41	kJ/mol	Joback Method
hvap	97.62	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	7.990		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	832.42	kPa	Joback Method
rinpol	2943.00		NIST Webbook
rinpol	2943.00		NIST Webbook
tb	1022.52	K	Joback Method
tc	1253.03	K	Joback Method
tf	528.58	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.70	J/mol×K	1022.52	Joback Method
cpg	1388.35	J/mol×K	1060.94	Joback Method
cpg	1404.22	J/mol×K	1099.36	Joback Method
cpg	1418.37	J/mol×K	1137.77	Joback Method
cpg	1430.88	J/mol×K	1176.19	Joback Method
cpg	1441.80	J/mol×K	1214.61	Joback Method
cpg	1451.20	J/mol×K	1253.03	Joback Method
dvisc	0.0003741	Pa×s	528.58	Joback Method

dvisc	0.0001414	Pa×s	610.90	Joback Method
dvisc	0.0000673	Pa×s	693.23	Joback Method
dvisc	0.0000375	Pa×s	775.55	Joback Method
dvisc	0.0000234	Pa×s	857.87	Joback Method
dvisc	0.0000158	Pa×s	940.20	Joback Method
dvisc	0.0000114	Pa×s	1022.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344680&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

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