Isophthalic acid, 6-ethyloct-3-yl isohexyl ester

Inchi: InChI=1S/C24H38O4/c1-6-19(7-2)14-15-22(8-3)28-24(26)21-13-9-12-20(17-21)23(25)27
InchiKey: RYKVEEOGIKQZSH-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCC(CC)CCC(CC)OC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-221.18	kJ/mol	Joback Method
hf	-819.07	kJ/mol	Joback Method
hfus	46.57	kJ/mol	Joback Method
hvap	89.10	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.431		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1047.33	kPa	Joback Method
rinpol	2704.00		NIST Webbook
rinpol	2704.00		NIST Webbook
tb	931.44	K	Joback Method
tc	1142.65	K	Joback Method
tf	498.50	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.72	J/mol×K	931.44	Joback Method
cpg	1192.10	J/mol×K	1107.45	Joback Method
cpg	1180.51	J/mol×K	1072.25	Joback Method
cpg	1167.62	J/mol×K	1037.04	Joback Method
cpg	1153.38	J/mol×K	1001.84	Joback Method
cpg	1137.76	J/mol×K	966.64	Joback Method
cpg	1202.41	J/mol×K	1142.65	Joback Method
dvisc	0.0000234	Pa×s	931.44	Joback Method

dvisc	0.0000318	Pa×s	859.28	Joback Method
dvisc	0.0000457	Pa×s	787.13	Joback Method
dvisc	0.0000707	Pa×s	714.97	Joback Method
dvisc	0.0001206	Pa×s	642.81	Joback Method
dvisc	0.0002354	Pa×s	570.66	Joback Method
dvisc	0.0005581	Pa×s	498.50	Joback Method

Sources

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=U344679&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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