Isophthalic acid, cyclohexylmethyl octyl ester

Inchi: InChI=1S/C23H34O4/c1-2-3-4-5-6-10-16-26-22(24)20-14-11-15-21(17-20)23(25)27-18-1
InchiKey: VENYVHVGGBJPEV-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-197.83	kJ/mol	Joback Method
hf	-728.27	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	88.47	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.941		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tb	929.43	K	Joback Method
tc	1147.80	K	Joback Method
tf	539.61	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.39	J/mol×K	929.43	Joback Method
cpg	1070.16	J/mol×K	965.82	Joback Method
cpg	1085.35	J/mol×K	1002.22	Joback Method
cpg	1099.02	J/mol×K	1038.61	Joback Method
cpg	1111.19	J/mol×K	1075.01	Joback Method
cpg	1121.93	J/mol×K	1111.40	Joback Method
cpg	1131.26	J/mol×K	1147.80	Joback Method
dvisc	0.0004850	Pa×s	539.61	Joback Method

dvisc	0.0002504	Pa×s	604.58	Joback Method
dvisc	0.0001470	Pa×s	669.55	Joback Method
dvisc	0.0000948	Pa×s	734.52	Joback Method
dvisc	0.0000657	Pa×s	799.49	Joback Method
dvisc	0.0000481	Pa×s	864.46	Joback Method
dvisc	0.0000368	Pa×s	929.43	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=U343830&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