Isophthalic acid, (2-chlorocyclohexyl)methyl hexyl ester

Inchi: InChI=1S/C21H29ClO4/c1-2-3-4-7-13-25-20(23)16-10-8-11-17(14-16)21(24)26-15-18-9-5

InchiKey: DFGLBZXEJUFHPG-UHFFFAOYSA-N

Formula: C21H29ClO4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2Cl)c1

Mol. weight [g/mol]: 380.91

Physical Properties

Property code	Value	Unit	Source
gf	-234.31	kJ/mol	Joback Method
hf	-723.07	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	88.09	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.378		Crippen Method
mcvol	299.250	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	916.43	K	Joback Method
tc	1138.56	K	Joback Method
tf	542.75	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.16	J/mol×K	916.43	Joback Method
cpg	978.80	J/mol×K	953.45	Joback Method
cpg	992.85	J/mol×K	990.47	Joback Method
cpg	1005.35	J/mol×K	1027.49	Joback Method
cpg	1016.33	J/mol×K	1064.52	Joback Method
cpg	1025.83	J/mol×K	1101.54	Joback Method
cpg	1033.86	J/mol×K	1138.56	Joback Method
dvisc	0.0005505	Pa×s	542.75	Joback Method

dvisc	0.0003084	Pa×s	605.03	Joback Method
dvisc	0.0001925	Pa×s	667.31	Joback Method
dvisc	0.0001303	Pa×s	729.59	Joback Method
dvisc	0.0000937	Pa×s	791.87	Joback Method
dvisc	0.0000707	Pa×s	854.15	Joback Method
dvisc	0.0000555	Pa×s	916.43	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=U343797&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