Phthalic acid, 2,2-dichloroethyl hexyl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-2-3-4-7-10-21-15(19)12-8-5-6-9-13(12)16(20)22-11-14(17)18
InchiKey: KTXDWQQJMPQCKJ-UHFFFAOYSA-N
Formula: C16H20Cl2O4
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-307.52	kJ/mol	Joback Method
hf	-674.87	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	80.84	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.384		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2314.00		NIST Webbook
tb	824.14	K	Joback Method
tc	1036.24	K	Joback Method
tf	498.18	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.68	J/mol×K	824.14	Joback Method
cpg	713.70	J/mol×K	859.49	Joback Method
cpg	725.67	J/mol×K	894.84	Joback Method
cpg	736.63	J/mol×K	930.19	Joback Method
cpg	746.58	J/mol×K	965.54	Joback Method
cpg	755.55	J/mol×K	1000.89	Joback Method
cpg	763.55	J/mol×K	1036.24	Joback Method
dvisc	0.0006699	Pa×s	498.18	Joback Method
dvisc	0.0003768	Pa×s	552.51	Joback Method

dvisc	0.0002349	Pa×s	606.83	Joback Method
dvisc	0.0001583	Pa×s	661.16	Joback Method
dvisc	0.0001132	Pa×s	715.49	Joback Method
dvisc	0.0000849	Pa×s	769.81	Joback Method
dvisc	0.0000662	Pa×s	824.14	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=U356927&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