Isophthalic acid, monochloride, cyclohexylmethyl ester

Inchi: InChI=1S/C15H17ClO3/c16-14(17)12-7-4-8-13(9-12)15(18)19-10-11-5-2-1-3-6-11/h4,7-9

InchiKey: OKVMSFMEFZQYOJ-UHFFFAOYSA-N

Formula: C15H17ClO3

SMILES: O=C(Cl)c1cccc(C(=O)OCC2CCCCC2)c1

Mol. weight [g/mol]: 280.75

Physical Properties

Property code	Value	Unit	Source
gf	-172.12	kJ/mol	Joback Method
hf	-446.67	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	72.64	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.803		Crippen Method
mcvol	208.840	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	761.40	K	Joback Method
tc	1000.82	K	Joback Method
tf	457.14	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.96	J/mol×K	761.40	Joback Method
cpg	652.25	J/mol×K	960.91	Joback Method
cpg	641.60	J/mol×K	921.01	Joback Method
cpg	629.69	J/mol×K	881.11	Joback Method
cpg	616.47	J/mol×K	841.21	Joback Method
cpg	601.91	J/mol×K	801.30	Joback Method
cpg	661.69	J/mol×K	1000.82	Joback Method
dvisc	0.0001295	Pa×s	761.40	Joback Method

dvisc	0.0001654	Pa×s	710.69	Joback Method
dvisc	0.0002195	Pa×s	659.98	Joback Method
dvisc	0.0003052	Pa×s	609.27	Joback Method
dvisc	0.0004507	Pa×s	558.56	Joback Method
dvisc	0.0007193	Pa×s	507.85	Joback Method
dvisc	0.0012734	Pa×s	457.14	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=U343836&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