

Isophthalic acid, butyl 2-chloroethyl ester

Inchi:	InChI=1S/C14H17ClO4/c1-2-3-8-18-13(16)11-5-4-6-12(10-11)14(17)19-9-7-15/h4-6,10H,
InchiKey:	LYGAXOOCKBINHY-UHFFFAOYSA-N
Formula:	C14H17ClO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OCCCl)c1
Mol. weight [g/mol]:	284.74

Physical Properties

Property code	Value	Unit	Source
gf	-309.99	kJ/mol	Joback Method
hf	-612.57	kJ/mol	Joback Method
hfus	35.44	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.039		Crippen Method
mvol	211.480	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	741.39	K	Joback Method
tc	950.76	K	Joback Method
tf	460.72	K	Joback Method
vc	0.808	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.99	J/molxK	741.39	Joback Method
cpg	623.52	J/molxK	915.86	Joback Method
cpg	613.81	J/molxK	880.97	Joback Method
cpg	603.21	J/molxK	846.07	Joback Method
cpg	591.71	J/molxK	811.18	Joback Method
cpg	579.31	J/molxK	776.28	Joback Method
cpg	632.35	J/molxK	950.76	Joback Method
dvisc	0.0001076	Paxs	741.39	Joback Method

dvisc	0.0001353	Paxs	694.61	Joback Method
dvisc	0.0001757	Paxs	647.83	Joback Method
dvisc	0.0002378	Paxs	601.06	Joback Method
dvisc	0.0003387	Paxs	554.28	Joback Method
dvisc	0.0005150	Paxs	507.50	Joback Method
dvisc	0.0008524	Paxs	460.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U345869&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

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