

Isophthalic acid, 2-chloroethyl heptyl ester

Inchi:	InChI=1S/C17H23ClO4/c1-2-3-4-5-6-11-21-16(19)14-8-7-9-15(13-14)17(20)22-12-10-18
InchiKey:	BKFZIAUFPIXTNT-UHFFFAOYSA-N
Formula:	C17H23ClO4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OCCCl)c1
Mol. weight [g/mol]:	326.81

Physical Properties

Property code	Value	Unit	Source
gf	-284.73	kJ/mol	Joback Method
hf	-674.49	kJ/mol	Joback Method
hfus	43.21	kJ/mol	Joback Method
hvap	79.07	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.209		Crippen Method
mvol	253.750	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2471.00		NIST Webbook
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tb	810.03	K	Joback Method
tc	1014.58	K	Joback Method
tf	494.53	K	Joback Method
vc	0.977	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.34	J/molxK	810.03	Joback Method
cpg	745.62	J/molxK	844.12	Joback Method
cpg	758.88	J/molxK	878.21	Joback Method
cpg	771.12	J/molxK	912.30	Joback Method
cpg	782.38	J/molxK	946.39	Joback Method
cpg	792.66	J/molxK	980.49	Joback Method
cpg	801.99	J/molxK	1014.58	Joback Method
dvisc	0.0006561	Paxs	494.53	Joback Method

dvisc	0.0003807	Paxs	547.11	Joback Method
dvisc	0.0002430	Paxs	599.70	Joback Method
dvisc	0.0001667	Paxs	652.28	Joback Method
dvisc	0.0001210	Paxs	704.86	Joback Method
dvisc	0.0000918	Paxs	757.45	Joback Method
dvisc	0.0000722	Paxs	810.03	Joback Method

Sources

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=U345872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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