

Isophthalic acid, 2-chloropropyl heptyl ester

Inchi:	InChI=1S/C18H25ClO4/c1-3-4-5-6-7-11-22-17(20)15-9-8-10-16(12-15)18(21)23-13-14(2)
InchiKey:	ZHUIXKTZQCXDPO-UHFFFAOYSA-N
Formula:	C18H25ClO4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OCC(C)Cl)c1
Mol. weight [g/mol]:	340.84

Physical Properties

Property code	Value	Unit	Source
gf	-278.75	kJ/mol	Joback Method
hf	-700.41	kJ/mol	Joback Method
hfus	42.28	kJ/mol	Joback Method
hvap	80.91	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.598		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2442.00		NIST Webbook
tb	832.47	K	Joback Method
tc	1038.76	K	Joback Method
tf	490.80	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.94	J/molxK	832.47	Joback Method
cpg	803.61	J/molxK	866.85	Joback Method
cpg	817.18	J/molxK	901.23	Joback Method
cpg	829.67	J/molxK	935.62	Joback Method
cpg	841.11	J/molxK	970.00	Joback Method
cpg	851.52	J/molxK	1004.38	Joback Method
cpg	860.90	J/molxK	1038.76	Joback Method
dvisc	0.0006700	Paxs	490.80	Joback Method
dvisc	0.0003599	Paxs	547.75	Joback Method

dvisc	0.0002174	Paxs	604.69	Joback Method
dvisc	0.0001432	Paxs	661.63	Joback Method
dvisc	0.0001008	Paxs	718.58	Joback Method
dvisc	0.0000747	Paxs	775.52	Joback Method
dvisc	0.0000577	Paxs	832.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356361&Units=SI
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

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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