

Isophthalic acid, 2-chloropropyl octyl ester

Inchi:	InChI=1S/C19H27ClO4/c1-3-4-5-6-7-8-12-23-18(21)16-10-9-11-17(13-16)19(22)24-14-15
InchiKey:	UEPRZLTVNDRJJD-UHFFFAOYSA-N
Formula:	C19H27ClO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)Cl)c1
Mol. weight [g/mol]:	354.87

Physical Properties

Property code	Value	Unit	Source
gf	-270.33	kJ/mol	Joback Method
hf	-721.05	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	83.14	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.988		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2542.00		NIST Webbook
tb	855.35	K	Joback Method
tc	1061.57	K	Joback Method
tf	502.07	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.82	J/molxK	855.35	Joback Method
cpg	861.69	J/molxK	889.72	Joback Method
cpg	875.42	J/molxK	924.09	Joback Method
cpg	888.04	J/molxK	958.46	Joback Method
cpg	899.57	J/molxK	992.83	Joback Method
cpg	910.03	J/molxK	1027.20	Joback Method
cpg	919.45	J/molxK	1061.57	Joback Method
dvisc	0.0006030	Paxs	502.07	Joback Method
dvisc	0.0003202	Paxs	560.95	Joback Method

dvisc	0.0001918	Paxs	619.83	Joback Method
dvisc	0.0001256	Paxs	678.71	Joback Method
dvisc	0.0000879	Paxs	737.59	Joback Method
dvisc	0.0000649	Paxs	796.47	Joback Method
dvisc	0.0000500	Paxs	855.35	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=U356362&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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