

Fumaric acid, 2-chloropropyl dodecyl ester

Inchi:	InChI=1S/C19H33ClO4/c1-3-4-5-6-7-8-9-10-11-12-15-23-18(21)13-14-19(22)24-16-17(2)
InchiKey:	KBMFXYTIXLVHL-BUHFOSPRSA-N
Formula:	C19H33ClO4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OCC(C)Cl
Mol. weight [g/mol]:	360.92

Physical Properties

Property code	Value	Unit	Source
gf	-292.89	kJ/mol	Joback Method
hf	-828.89	kJ/mol	Joback Method
hfus	51.42	kJ/mol	Joback Method
hvap	80.16	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.177		Crippen Method
mvol	301.390	ml/mol	McGowan Method
pc	1167.22	kPa	Joback Method
rinpol	2473.00		NIST Webbook
tb	827.85	K	Joback Method
tc	1018.82	K	Joback Method
tf	458.05	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.20	J/molxK	827.85	Joback Method
cpg	987.90	J/molxK	986.99	Joback Method
cpg	975.23	J/molxK	955.17	Joback Method
cpg	961.65	J/molxK	923.34	Joback Method
cpg	947.14	J/molxK	891.51	Joback Method
cpg	931.66	J/molxK	859.68	Joback Method
cpg	999.69	J/molxK	1018.82	Joback Method
dvisc	0.0000422	Paxs	827.85	Joback Method
dvisc	0.0000566	Paxs	766.22	Joback Method

dvisc	0.0000800	Paxs	704.58	Joback Method
dvisc	0.0001206	Paxs	642.95	Joback Method
dvisc	0.0001985	Paxs	581.32	Joback Method
dvisc	0.0003677	Paxs	519.68	Joback Method
dvisc	0.0008039	Paxs	458.05	Joback Method

Sources

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=U348570&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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