

Fumaric acid, 2,2-dichloroethyl dodecyl ester

Inchi:	InChI=1S/C18H30Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-14-23-17(21)12-13-18(22)24-15-16(19)
InchiKey:	IDWSWXWSQPMUQF-OUKQBFOZSA-N
Formula:	C18H30Cl2O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	381.33

Physical Properties

Property code	Value	Unit	Source
gf	-313.24	kJ/mol	Joback Method
hf	-823.99	kJ/mol	Joback Method
hfus	53.02	kJ/mol	Joback Method
hvap	82.31	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.354		Crippen Method
mvol	299.540	ml/mol	McGowan Method
pc	1215.74	kPa	Joback Method
rinpol	2533.00		NIST Webbook
tb	842.40	K	Joback Method
tc	1037.35	K	Joback Method
tf	476.70	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.73	J/molxK	842.40	Joback Method
cpg	899.88	J/molxK	874.89	Joback Method
cpg	914.07	J/molxK	907.38	Joback Method
cpg	927.33	J/molxK	939.87	Joback Method
cpg	939.68	J/molxK	972.36	Joback Method
cpg	951.16	J/molxK	1004.85	Joback Method
cpg	961.79	J/molxK	1037.35	Joback Method
dvisc	0.0007015	Paxs	476.70	Joback Method
dvisc	0.0003358	Paxs	537.65	Joback Method

dvisc	0.0001867	Paxs	598.60	Joback Method
dvisc	0.0001157	Paxs	659.55	Joback Method
dvisc	0.0000778	Paxs	720.50	Joback Method
dvisc	0.0000556	Paxs	781.45	Joback Method
dvisc	0.0000417	Paxs	842.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U348580&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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