Fumaric acid, 2,2-dichloroethyl undecyl ester

Inchi: InChI=1S/C17H28Cl2O4/c1-2-3-4-5-6-7-8-9-10-13-22-16(20)11-12-17(21)23-14-15(18)19
InchiKey: QRWWZUHTBJNFPP-VAWYXSNFSA-N
Formula: C17H28Cl2O4
SMILES: CCCCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 367.31

Physical Properties

Property code	Value	Unit	Source
gf	-321.66	kJ/mol	Joback Method
hf	-803.35	kJ/mol	Joback Method
hfus	50.43	kJ/mol	Joback Method
hvap	80.09	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.964		Crippen Method
mcvol	285.450	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
rinpol	2434.00		NIST Webbook
rinpol	2434.00		NIST Webbook
tb	819.52	K	Joback Method
tc	1012.86	K	Joback Method
tf	465.43	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.51	J/mol×K	819.52	Joback Method
cpg	841.29	J/mol×K	851.74	Joback Method
cpg	855.16	J/mol×K	883.97	Joback Method
cpg	868.14	J/mol×K	916.19	Joback Method
cpg	880.26	J/mol×K	948.41	Joback Method
cpg	891.53	J/mol×K	980.64	Joback Method
cpg	901.99	J/mol×K	1012.86	Joback Method
dvisc	0.0007883	Pa×s	465.43	Joback Method

dvisc	0.0003813	Pa×s	524.44	Joback Method
dvisc	0.0002136	Pa×s	583.46	Joback Method
dvisc	0.0001331	Pa×s	642.47	Joback Method
dvisc	0.0000898	Pa×s	701.49	Joback Method
dvisc	0.0000644	Pa×s	760.50	Joback Method
dvisc	0.0000485	Pa×s	819.52	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=U348579&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