Fumaric acid, 2,2-dichloroethyl pentadecyl ester

Inchi: InChI=1S/C21H36Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-26-20(24)15-16-21(25)27
InchiKey: MWXYEQDJMAXBGQ-FOCLMDBBSA-N
Formula: C21H36Cl2O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 423.41

Physical Properties

Property code	Value	Unit	Source
gf	-287.98	kJ/mol	Joback Method
hf	-885.91	kJ/mol	Joback Method
hfus	60.79	kJ/mol	Joback Method
hvap	88.99	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.524		Crippen Method
mcvol	341.810	ml/mol	McGowan Method
pc	1003.98	kPa	Joback Method
rinpol	2827.00		NIST Webbook
tb	911.04	K	Joback Method
tc	1115.57	K	Joback Method
tf	510.51	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.07	J/mol×K	911.04	Joback Method
cpg	1134.70	J/mol×K	1081.48	Joback Method
cpg	1122.68	J/mol×K	1047.39	Joback Method
cpg	1109.64	J/mol×K	1013.30	Joback Method
cpg	1095.56	J/mol×K	979.22	Joback Method
cpg	1080.38	J/mol×K	945.13	Joback Method
cpg	1145.76	J/mol×K	1115.57	Joback Method
dvisc	0.0000264	Pa×s	911.04	Joback Method
dvisc	0.0000354	Pa×s	844.28	Joback Method

dvisc	0.0000499	Pa×s	777.53	Joback Method
dvisc	0.0000750	Pa×s	710.77	Joback Method
dvisc	0.0001228	Pa×s	644.02	Joback Method
dvisc	0.0002254	Pa×s	577.26	Joback Method
dvisc	0.0004848	Pa×s	510.51	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=U348582&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