Fumaric acid, decyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C16H26Cl2O4/c1-2-3-4-5-6-7-8-9-12-21-15(19)10-11-16(20)22-13-14(17)18/h1
InchiKey: LAROUSPUHKQQBD-ZHACJKMWSA-N
Formula: C16H26Cl2O4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 353.28

Physical Properties

Property code	Value	Unit	Source
gf	-330.08	kJ/mol	Joback Method
hf	-782.71	kJ/mol	Joback Method
hfus	47.84	kJ/mol	Joback Method
hvap	77.86	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.573		Crippen Method
mcvol	271.360	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	2336.00		NIST Webbook
tb	796.64	K	Joback Method
tc	989.07	K	Joback Method
tf	454.16	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.17	J/mol×K	796.64	Joback Method
cpg	832.73	J/mol×K	957.00	Joback Method
cpg	821.67	J/mol×K	924.93	Joback Method
cpg	809.82	J/mol×K	892.86	Joback Method
cpg	797.13	J/mol×K	860.78	Joback Method
cpg	783.59	J/mol×K	828.71	Joback Method
cpg	843.00	J/mol×K	989.07	Joback Method
dvisc	0.0000561	Pa×s	796.64	Joback Method
dvisc	0.0000744	Pa×s	739.56	Joback Method

dvisc	0.0001034	Pa×s	682.48	Joback Method
dvisc	0.0001527	Pa×s	625.40	Joback Method
dvisc	0.0002436	Pa×s	568.32	Joback Method
dvisc	0.0004315	Pa×s	511.24	Joback Method
dvisc	0.0008825	Pa×s	454.16	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=U348578&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