Fumaric acid, 2,2-dichloroethyl pentyl ester

Inchi: InChI=1S/C11H16Cl2O4/c1-2-3-4-7-16-10(14)5-6-11(15)17-8-9(12)13/h5-6,9H,2-4,7-8H2
InchiKey: XMQDRXJXGJNOAC-AATRIKPKSA-N
Formula: C11H16Cl2O4
SMILES: CCCCCOC(=O)C=CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 283.15

Physical Properties

Property code	Value	Unit	Source
gf	-372.18	kJ/mol	Joback Method
hf	-679.51	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	66.73	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.623		Crippen Method
mcvol	200.910	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1821.00		NIST Webbook
rinpol	1821.00		NIST Webbook
tb	682.24	K	Joback Method
tc	878.76	K	Joback Method
tf	397.81	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.46	J/mol×K	682.24	Joback Method
cpg	510.59	J/mol×K	714.99	Joback Method
cpg	522.03	J/mol×K	747.75	Joback Method
cpg	532.79	J/mol×K	780.50	Joback Method
cpg	542.89	J/mol×K	813.25	Joback Method
cpg	552.34	J/mol×K	846.01	Joback Method
cpg	561.14	J/mol×K	878.76	Joback Method
dvisc	0.0014520	Pa×s	397.81	Joback Method

dvisc	0.0007558	Pa×s	445.22	Joback Method
dvisc	0.0004461	Pa×s	492.62	Joback Method
dvisc	0.0002888	Pa×s	540.02	Joback Method
dvisc	0.0002006	Pa×s	587.43	Joback Method
dvisc	0.0001471	Pa×s	634.84	Joback Method
dvisc	0.0001126	Pa×s	682.24	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=U348576&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