Fumaric acid, naphth-2-yl 2,2-dichloroethyl ester

Inchi: InChI=1S/C16H12Cl2O4/c17-14(18)10-21-15(19)7-8-16(20)22-13-6-5-11-3-1-2-4-12(11)9

InchiKey: ZUXDFJBCQQSUIG-BQYQJAHWSA-N

Formula: C16H12Cl2O4

SMILES: O=C(C=CC(=O)Oc1ccc2ccccc2c1)OCC(Cl)Cl

Mol. weight [g/mol]: 339.17

Physical Properties

Property code	Value	Unit	Source
gf	-120.65	kJ/mol	Joback Method
hf	-366.58	kJ/mol	Joback Method
hfus	38.51	kJ/mol	Joback Method
hvap	82.44	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.648		Crippen Method
mcvol	228.140	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	847.28	K	Joback Method
tc	1085.54	K	Joback Method
tf	525.80	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.34	J/mol×K	847.28	Joback Method
cpg	642.75	J/mol×K	1045.83	Joback Method
cpg	635.20	J/mol×K	1006.12	Joback Method
cpg	626.95	J/mol×K	966.41	Joback Method
cpg	617.94	J/mol×K	926.70	Joback Method
cpg	608.10	J/mol×K	886.99	Joback Method
cpg	649.70	J/mol×K	1085.54	Joback Method
dvisc	0.0001131	Pa×s	847.28	Joback Method

dvisc	0.0001391	Pa×s	793.70	Joback Method
dvisc	0.0001763	Pa×s	740.12	Joback Method
dvisc	0.0002317	Pa×s	686.54	Joback Method
dvisc	0.0003191	Pa×s	632.96	Joback Method
dvisc	0.0004662	Pa×s	579.38	Joback Method
dvisc	0.0007359	Pa×s	525.80	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=U405827&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