

Fumaric acid, naphth-1-yl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C16H12Cl2O4/c17-14(18)10-21-15(19)8-9-16(20)22-13-7-3-5-11-4-1-2-6-12(1
InchiKey:	FJKJSQYRSRXTKJ-CMDGGOBGSA-N
Formula:	C16H12Cl2O4
SMILES:	O=C(C=CC(=O)Oc1cccc2ccccc12)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
mvol	228.140	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	2559.00		NIST Webbook
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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/molxK	847.28	Joback Method
cpg	608.10	J/molxK	886.99	Joback Method
cpg	617.94	J/molxK	926.70	Joback Method
cpg	626.95	J/molxK	966.41	Joback Method
cpg	635.20	J/molxK	1006.12	Joback Method
cpg	642.75	J/molxK	1045.83	Joback Method
cpg	649.70	J/molxK	1085.54	Joback Method
dvisc	0.0007359	Paxs	525.80	Joback Method

dvisc	0.0004662	Paxs	579.38	Joback Method
dvisc	0.0003191	Paxs	632.96	Joback Method
dvisc	0.0002317	Paxs	686.54	Joback Method
dvisc	0.0001763	Paxs	740.12	Joback Method
dvisc	0.0001391	Paxs	793.70	Joback Method
dvisc	0.0001131	Paxs	847.28	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=U405808&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

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