

Fumaric acid, 2,6-dichlorophenyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C21H14Cl2O4/c22-17-6-3-7-18(23)21(17)27-20(25)11-10-19(24)26-13-14-8-9-
InchiKey: CFXNDCCIFYYYCM-ZHACJKMWSA-N
Formula: C21H14Cl2O4
SMILES: O=C(C=CC(=O)Oc1c(Cl)cccc1Cl)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 401.24

Physical Properties

Property code	Value	Unit	Source
gf	17.04	kJ/mol	Joback Method
hf	-250.91	kJ/mol	Joback Method
hfus	48.25	kJ/mol	Joback Method
hvap	97.56	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.352		Crippen Method
mvol	274.830	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	3140.00		NIST Webbook
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tb	998.76	K	Joback Method
tc	1252.56	K	Joback Method
tf	648.61	K	Joback Method
vc	1.044	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.47	J/molxK	998.76	Joback Method
cpg	808.68	J/molxK	1210.26	Joback Method
cpg	801.61	J/molxK	1167.96	Joback Method
cpg	793.96	J/molxK	1125.66	Joback Method
cpg	785.63	J/molxK	1083.36	Joback Method
cpg	776.50	J/molxK	1041.06	Joback Method
cpg	815.27	J/molxK	1252.56	Joback Method
dvisc	0.0000694	Paxs	998.76	Joback Method

dvisc	0.0000834	Paxs	940.40	Joback Method
dvisc	0.0001027	Paxs	882.04	Joback Method
dvisc	0.0001302	Paxs	823.68	Joback Method
dvisc	0.0001712	Paxs	765.33	Joback Method
dvisc	0.0002356	Paxs	706.97	Joback Method
dvisc	0.0003433	Paxs	648.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405866&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

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