Fumaric acid, 2,4-dichlorophenyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C21H14Cl2O4/c22-17-7-8-19(18(23)12-17)27-21(25)10-9-20(24)26-13-14-5-6-

InchiKey: RYVXWIBEEIYSNF-MDZDMXLPSA-N

Formula: C21H14Cl2O4

SMILES: O=C(C=CC(=O)Oc1ccc(Cl)cc1Cl)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
mcvol	274.830	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	998.76	K	Joback Method
tc	1252.56	K	Joback Method
tf	648.61	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.47	J/mol×K	998.76	Joback Method
cpg	776.50	J/mol×K	1041.06	Joback Method
cpg	785.63	J/mol×K	1083.36	Joback Method
cpg	793.96	J/mol×K	1125.66	Joback Method
cpg	801.61	J/mol×K	1167.96	Joback Method
cpg	808.68	J/mol×K	1210.26	Joback Method
cpg	815.27	J/mol×K	1252.56	Joback Method
dvisc	0.0003433	Pa×s	648.61	Joback Method

dvisc	0.0002356	Pa×s	706.97	Joback Method
dvisc	0.0001712	Pa×s	765.33	Joback Method
dvisc	0.0001302	Pa×s	823.68	Joback Method
dvisc	0.0001027	Pa×s	882.04	Joback Method
dvisc	0.0000834	Pa×s	940.40	Joback Method
dvisc	0.0000694	Pa×s	998.76	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=U405706&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