Fumaric acid, naphth-1-yl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C20H12Cl2O4/c21-15-8-4-10-17(20(15)22)26-19(24)12-11-18(23)25-16-9-3-6-

InchiKey: IIZDNOZTVZYROQ-VAWYXSNFSA-N

Formula: C20H12Cl2O4

SMILES: O=C(C=CC(=O)Oc1cccc2ccccc12)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 387.21

Physical Properties

Property code	Value	Unit	Source
gf	8.62	kJ/mol	Joback Method
hf	-230.27	kJ/mol	Joback Method
hfus	45.66	kJ/mol	Joback Method
hvap	95.33	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.214		Crippen Method
mcvol	260.740	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	3125.00		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	975.88	K	Joback Method
tc	1232.56	K	Joback Method
tf	637.34	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.58	J/mol×K	975.88	Joback Method
cpg	750.17	J/mol×K	1189.78	Joback Method
cpg	743.46	J/mol×K	1147.00	Joback Method
cpg	736.15	J/mol×K	1104.22	Joback Method
cpg	728.14	J/mol×K	1061.44	Joback Method
cpg	719.32	J/mol×K	1018.66	Joback Method
cpg	756.38	J/mol×K	1232.56	Joback Method
dvisc	0.0000795	Pa×s	975.88	Joback Method

dvisc	0.0000952	Pa×s	919.46	Joback Method
dvisc	0.0001167	Pa×s	863.03	Joback Method
dvisc	0.0001472	Pa×s	806.61	Joback Method
dvisc	0.0001923	Pa×s	750.19	Joback Method
dvisc	0.0002623	Pa×s	693.76	Joback Method
dvisc	0.0003781	Pa×s	637.34	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=U405816&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