Fumaric acid, naphth-1-yl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C20H11Cl3O4/c21-13-10-15(22)20(16(23)11-13)27-19(25)9-8-18(24)26-17-7-3

InchiKey: SHPOCXLCCDDZBJ-CMDGGOBGSA-N

Formula: C20H11Cl3O4

SMILES: O=C(C=CC(=O)Oc1cccc2ccccc12)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 421.66

Physical Properties

Property code	Value	Unit	Source
gf	-12.94	kJ/mol	Joback Method
hf	-257.48	kJ/mol	Joback Method
hfus	49.47	kJ/mol	Joback Method
hvap	100.38	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	5.867		Crippen Method
mcvol	272.980	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	3119.00		NIST Webbook
rinpol	3119.00		NIST Webbook
tb	1018.29	K	Joback Method
tc	1278.09	K	Joback Method
tf	679.78	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.34	J/mol×K	1018.29	Joback Method
cpg	732.95	J/mol×K	1061.59	Joback Method
cpg	740.72	J/mol×K	1104.89	Joback Method
cpg	747.75	J/mol×K	1148.19	Joback Method
cpg	754.14	J/mol×K	1191.49	Joback Method
cpg	759.99	J/mol×K	1234.79	Joback Method
cpg	765.39	J/mol×K	1278.09	Joback Method
dvisc	0.0003038	Pa×s	679.78	Joback Method

dvisc	0.0002170	Pa×s	736.20	Joback Method
dvisc	0.0001626	Pa×s	792.62	Joback Method
dvisc	0.0001266	Pa×s	849.04	Joback Method
dvisc	0.0001017	Pa×s	905.45	Joback Method
dvisc	0.0000838	Pa×s	961.87	Joback Method
dvisc	0.0000706	Pa×s	1018.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405818&Units=SI
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

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