

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

Inchi: InChI=1S/C20H11Cl3O4/c21-14-10-16(22)20(17(23)11-14)27-19(25)8-7-18(24)26-15-6-5
InchiKey: BYYLOIXMTNKTQP-BQYQJAHWSA-N
Formula: C20H11Cl3O4
SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccc2ccccc2c1
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	3156.00		NIST Webbook
rinpol	3156.00		NIST Webbook
tb	1018.29	K	Joback Method
tc	1278.09	K	Joback Method
tf	679.78	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002170	Paxs	736.20	Joback Method
dvisc	0.0001626	Paxs	792.62	Joback Method
dvisc	0.0001266	Paxs	849.04	Joback Method
dvisc	0.0001017	Paxs	905.45	Joback Method
dvisc	0.0000838	Paxs	961.87	Joback Method
dvisc	0.0000706	Paxs	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=U405836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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