

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

Inchi:	InChI=1S/C20H12Cl2O4/c21-16-6-3-7-17(20(16)22)26-19(24)11-10-18(23)25-15-9-8-13-
InchiKey:	FGCYEKDAGVUERL-ZHACJKMWSA-N
Formula:	C20H12Cl2O4
SMILES:	O=C(C=CC(=O)Oc1cccc(Cl)c1Cl)Oc1ccc2ccccc2c1
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
mvol	260.740	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	3125.00		NIST Webbook
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tb	975.88	K	Joback Method
tc	1232.56	K	Joback Method
tf	637.34	K	Joback Method
vc	0.988	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.58	J/molxK	975.88	Joback Method
cpg	719.32	J/molxK	1018.66	Joback Method
cpg	728.14	J/molxK	1061.44	Joback Method
cpg	736.15	J/molxK	1104.22	Joback Method
cpg	743.46	J/molxK	1147.00	Joback Method
cpg	750.17	J/molxK	1189.78	Joback Method
cpg	756.38	J/molxK	1232.56	Joback Method
dvisc	0.0003781	Paxs	637.34	Joback Method

dvisc	0.0002623	Paxs	693.76	Joback Method
dvisc	0.0001923	Paxs	750.19	Joback Method
dvisc	0.0001472	Paxs	806.61	Joback Method
dvisc	0.0001167	Paxs	863.03	Joback Method
dvisc	0.0000952	Paxs	919.46	Joback Method
dvisc	0.0000795	Paxs	975.88	Joback Method

Sources

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=U405834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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