

Fumaric acid, 2-chloro-5-methylphenyl nonyl ester

Inchi:	InChI=1S/C20H27ClO4/c1-3-4-5-6-7-8-9-14-24-19(22)12-13-20(23)25-18-15-16(2)10-11
InchiKey:	FGYSIMUZJAJGCJ-OUKQBFOZSA-N
Formula:	C20H27ClO4
SMILES:	CCCCCCCCCOC(=O)C=CC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	366.88

Physical Properties

Property code	Value	Unit	Source
gf	-188.88	kJ/mol	Joback Method
hf	-630.66	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	86.37	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.404		Crippen Method
mcvol	291.720	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook
tb	887.81	K	Joback Method
tc	1097.74	K	Joback Method
tf	535.78	K	Joback Method
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.67	J/molxK	887.81	Joback Method
cpg	938.50	J/molxK	1062.75	Joback Method
cpg	928.16	J/molxK	1027.76	Joback Method
cpg	916.85	J/molxK	992.78	Joback Method
cpg	904.52	J/molxK	957.79	Joback Method
cpg	891.14	J/molxK	922.80	Joback Method
cpg	947.88	J/molxK	1097.74	Joback Method
dvisc	0.0000420	Paxs	887.81	Joback Method

dvisc	0.0000534	Paxs	829.14	Joback Method
dvisc	0.0000704	Paxs	770.47	Joback Method
dvisc	0.0000971	Paxs	711.79	Joback Method
dvisc	0.0001419	Paxs	653.12	Joback Method
dvisc	0.0002236	Paxs	594.45	Joback Method
dvisc	0.0003892	Paxs	535.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U348261&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

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