

Fumaric acid, 3,5-dichlorophenyl propyl ester

Inchi: InChI=1S/C13H12Cl2O4/c1-2-5-18-12(16)3-4-13(17)19-11-7-9(14)6-10(15)8-11/h3-4,6-8
InchiKey: GQDYWAPQBXUEDV-ONEGZZNKSA-N
Formula: C13H12Cl2O4
SMILES: CCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 303.14

Physical Properties

Property code	Value	Unit	Source
gf	-259.75	kJ/mol	Joback Method
hf	-501.92	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	75.17	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.408		Crippen Method
mcvol	205.330	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpola	2100.00		NIST Webbook
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tb	765.08	K	Joback Method
tc	988.37	K	Joback Method
tf	486.81	K	Joback Method
vc	0.781	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.22	J/molxK	765.08	Joback Method
cpg	557.37	J/molxK	951.16	Joback Method
cpg	549.58	J/molxK	913.94	Joback Method
cpg	540.98	J/molxK	876.73	Joback Method
cpg	531.57	J/molxK	839.51	Joback Method
cpg	521.32	J/molxK	802.30	Joback Method
cpg	564.37	J/molxK	988.37	Joback Method
dvisc	0.0000948	Paxs	765.08	Joback Method

dvisc	0.0001172	Paxs	718.70	Joback Method
dvisc	0.0001493	Paxs	672.32	Joback Method
dvisc	0.0001972	Paxs	625.95	Joback Method
dvisc	0.0002721	Paxs	579.57	Joback Method
dvisc	0.0003973	Paxs	533.19	Joback Method
dvisc	0.0006233	Paxs	486.81	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=U348232&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

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