

Fumaric acid, 3-chlorophenyl 2-ethylhexyl ester

Inchi:	InChI=1S/C18H23ClO4/c1-3-5-7-14(4-2)13-22-17(20)10-11-18(21)23-16-9-6-8-15(19)12
InchiKey:	IILUXGQRWNAQSE-ZHACJKMWSA-N
Formula:	C18H23ClO4
SMILES:	CCCCC(CC)COC(=O)C=CC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	338.83

Physical Properties

Property code	Value	Unit	Source
gf	-198.53	kJ/mol	Joback Method
hf	-583.19	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.561		Crippen Method
mcvol	263.540	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2386.00		NIST Webbook
rinpol	2386.00		NIST Webbook
tb	836.63	K	Joback Method
tc	1048.04	K	Joback Method
tf	485.72	K	Joback Method
vc	1.006	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.42	J/molxK	836.63	Joback Method
cpg	776.62	J/molxK	871.86	Joback Method
cpg	789.77	J/molxK	907.10	Joback Method
cpg	801.91	J/molxK	942.33	Joback Method
cpg	813.06	J/molxK	977.57	Joback Method
cpg	823.27	J/molxK	1012.80	Joback Method
cpg	832.56	J/molxK	1048.04	Joback Method
dvisc	0.0006195	Paxs	485.72	Joback Method

dvisc	0.0003254	Paxs	544.21	Joback Method
dvisc	0.0001937	Paxs	602.69	Joback Method
dvisc	0.0001264	Paxs	661.17	Joback Method
dvisc	0.0000884	Paxs	719.66	Joback Method
dvisc	0.0000652	Paxs	778.14	Joback Method
dvisc	0.0000502	Paxs	836.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	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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