

Fumaric acid, hexyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C16H17Cl3O4/c1-2-3-4-5-8-22-14(20)6-7-15(21)23-11-9-12(17)16(19)13(18)10
InchiKey:	AEMQNCQCPLKIPB-VOTSOKGWSA-N
Formula:	C16H17Cl3O4
SMILES:	CCCCCCOC(=O)C=CC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	379.66

Physical Properties

Property code	Value	Unit	Source
gf	-256.05	kJ/mol	Joback Method
hf	-591.05	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.232		Crippen Method
mvol	259.840	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook
tb	876.13	K	Joback Method
tc	1096.52	K	Joback Method
tf	563.06	K	Joback Method
vc	0.999	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.67	J/molxK	876.13	Joback Method
cpg	703.79	J/molxK	912.86	Joback Method
cpg	713.96	J/molxK	949.59	Joback Method
cpg	723.20	J/molxK	986.32	Joback Method
cpg	731.53	J/molxK	1023.06	Joback Method
cpg	738.99	J/molxK	1059.79	Joback Method
cpg	745.58	J/molxK	1096.52	Joback Method
dvisc	0.0003567	Paxs	563.06	Joback Method

dvisc	0.0002296	Paxs	615.24	Joback Method
dvisc	0.0001584	Paxs	667.42	Joback Method
dvisc	0.0001153	Paxs	719.60	Joback Method
dvisc	0.0000876	Paxs	771.77	Joback Method
dvisc	0.0000689	Paxs	823.95	Joback Method
dvisc	0.0000558	Paxs	876.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348155&Units=SI
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

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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