Fumaric acid, hexyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C16H17Cl3O4/c1-2-3-4-5-10-22-13(20)8-9-14(21)23-16-12(18)7-6-11(17)15(16
InchiKey: VUMBEVNGFWMEEA-CMDGGOBGSA-N
Formula: C16H17Cl3O4
SMILES: CCCCCCOC(=O)C=CC(=O)Oc1c(Cl)ccc(Cl)c1Cl
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
mcvol	259.840	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	876.13	K	Joback Method
tc	1096.52	K	Joback Method
tf	563.06	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002296	Pa×s	615.24	Joback Method
dvisc	0.0001584	Pa×s	667.42	Joback Method
dvisc	0.0001153	Pa×s	719.60	Joback Method
dvisc	0.0000876	Pa×s	771.77	Joback Method
dvisc	0.0000689	Pa×s	823.95	Joback Method
dvisc	0.0000558	Pa×s	876.13	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=U348225&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

Latest version available from:
https://www.chemeo.com/cid/38-785-9/Fumaric-acid-hexyl-2-3-6-trichlorophenyl-ester.pdf
Generated by Cheméo on 2025-12-05 12:25:04.617401217 +0000 UTC m=+4685702.147441871.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.