

Fumaric acid, hexyl pentachlorophenyl ester

Inchi:	InChI=1S/C16H15Cl5O4/c1-2-3-4-5-8-24-9(22)6-7-10(23)25-16-14(20)12(18)11(17)13(19)
InchiKey:	HIPBUHXRIHIIST-VOTSOKGWSA-N
Formula:	C16H15Cl5O4
SMILES:	CCCCCOC(=O)C=CC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	448.55

Physical Properties

Property code	Value	Unit	Source
gf	-299.17	kJ/mol	Joback Method
hf	-645.47	kJ/mol	Joback Method
hfus	56.05	kJ/mol	Joback Method
hvap	96.99	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.539		Crippen Method
mcvol	284.320	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinsol	2919.00		NIST Webbook
tb	960.95	K	Joback Method
tc	1191.11	K	Joback Method
tf	647.94	K	Joback Method
vc	1.097	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.93	J/molxK	960.95	Joback Method
cpg	762.19	J/molxK	1152.75	Joback Method
cpg	757.24	J/molxK	1114.39	Joback Method
cpg	751.36	J/molxK	1076.03	Joback Method
cpg	744.52	J/molxK	1037.67	Joback Method
cpg	736.72	J/molxK	999.31	Joback Method
cpg	766.21	J/molxK	1191.11	Joback Method
dvisc	0.0000423	Paxs	960.95	Joback Method
dvisc	0.0000510	Paxs	908.78	Joback Method

dvisc	0.0000631	Paxs	856.61	Joback Method
dvisc	0.0000802	Paxs	804.45	Joback Method
dvisc	0.0001053	Paxs	752.28	Joback Method
dvisc	0.0001441	Paxs	700.11	Joback Method
dvisc	0.0002073	Paxs	647.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348184&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
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
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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