

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

Inchi:	InChI=1S/C16H17Cl3O4/c1-10(2)4-3-7-22-14(20)5-6-15(21)23-11-8-12(17)16(19)13(18)3
InchiKey:	HDCIXOJTYKFIFX-AATRIKPKSA-N
Formula:	C16H17Cl3O4
SMILES:	CC(C)CCCOC(=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	-258.49	kJ/mol	Joback Method
hf	-596.33	kJ/mol	Joback Method
hfus	44.91	kJ/mol	Joback Method
hvap	86.51	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.088		Crippen Method
mvol	259.840	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2578.00		NIST Webbook
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tb	875.69	K	Joback Method
tc	1098.72	K	Joback Method
tf	548.06	K	Joback Method
vc	0.993	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.24	J/molxK	875.69	Joback Method
cpg	704.46	J/molxK	912.86	Joback Method
cpg	714.70	J/molxK	950.03	Joback Method
cpg	723.97	J/molxK	987.20	Joback Method
cpg	732.30	J/molxK	1024.38	Joback Method
cpg	739.72	J/molxK	1061.55	Joback Method
cpg	746.25	J/molxK	1098.72	Joback Method
dvisc	0.0003853	Paxs	548.06	Joback Method

dvisc	0.0002361	Paxs	602.67	Joback Method
dvisc	0.0001570	Paxs	657.27	Joback Method
dvisc	0.0001111	Paxs	711.88	Joback Method
dvisc	0.0000826	Paxs	766.48	Joback Method
dvisc	0.0000639	Paxs	821.09	Joback Method
dvisc	0.0000510	Paxs	875.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348154&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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