

Fumaric acid, heptyl 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C17H19Cl3O4/c1-2-3-4-5-6-9-23-16(21)7-8-17(22)24-15-11-13(19)12(18)10-14
InchiKey:	IUMMUYUNAGBGY-BQYQJAHWSA-N
Formula:	C17H19Cl3O4
SMILES:	CCCCCCCOC(=O)C=CC(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	393.69

Physical Properties

Property code	Value	Unit	Source
gf	-247.63	kJ/mol	Joback Method
hf	-611.69	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	89.12	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.622		Crippen Method
mcvol	273.930	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2654.00		NIST Webbook
rinpol	2654.00		NIST Webbook
tb	899.01	K	Joback Method
tc	1118.59	K	Joback Method
tf	574.33	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.89	J/molxK	899.01	Joback Method
cpg	760.30	J/molxK	935.61	Joback Method
cpg	770.72	J/molxK	972.20	Joback Method
cpg	780.19	J/molxK	1008.80	Joback Method
cpg	788.72	J/molxK	1045.40	Joback Method
cpg	796.34	J/molxK	1082.00	Joback Method
cpg	803.09	J/molxK	1118.59	Joback Method
dvisc	0.0003225	Paxs	574.33	Joback Method

dvisc	0.0002051	Paxs	628.44	Joback Method
dvisc	0.0001402	Paxs	682.56	Joback Method
dvisc	0.0001013	Paxs	736.67	Joback Method
dvisc	0.0000766	Paxs	790.78	Joback Method
dvisc	0.0000600	Paxs	844.90	Joback Method
dvisc	0.0000484	Paxs	899.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348138&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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