

Glutaric acid, 2,4,6-trichlorophenyl 2-hexyl ester

Inchi:	InChI=1S/C17H21Cl3O4/c1-3-4-6-11(2)23-15(21)7-5-8-16(22)24-17-13(19)9-12(18)10-14
InchiKey:	NRXPYGLBIMZDMQ-UHFFFAOYSA-N
Formula:	C17H21Cl3O4
SMILES:	CCCCC(C)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	395.70

Physical Properties

Property code	Value	Unit	Source
gf	-330.29	kJ/mol	Joback Method
hf	-734.19	kJ/mol	Joback Method
hfus	47.30	kJ/mol	Joback Method
hvap	88.78	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.844		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
tb	894.41	K	Joback Method
tc	1111.41	K	Joback Method
tf	564.41	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.49	J/molxK	894.41	Joback Method
cpg	789.38	J/molxK	930.58	Joback Method
cpg	800.17	J/molxK	966.74	Joback Method
cpg	809.86	J/molxK	1002.91	Joback Method
cpg	818.46	J/molxK	1039.08	Joback Method
cpg	826.00	J/molxK	1075.25	Joback Method
cpg	832.48	J/molxK	1111.41	Joback Method
dvisc	0.0003779	Paxs	564.41	Joback Method

dvisc	0.0002328	Paxs	619.41	Joback Method
dvisc	0.0001552	Paxs	674.41	Joback Method
dvisc	0.0001100	Paxs	729.41	Joback Method
dvisc	0.0000818	Paxs	784.41	Joback Method
dvisc	0.0000633	Paxs	839.41	Joback Method
dvisc	0.0000505	Paxs	894.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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