

Glutaric acid, di(2,3,6-trichlorophenyl) ester

Inchi: InChI=1S/C17H10Cl6O4/c18-8-4-6-10(20)16(14(8)22)26-12(24)2-1-3-13(25)27-17-11(21)
InchiKey: PFAYVZPFHREBFJ-UHFFFAOYSA-N
Formula: C17H10Cl6O4
SMILES: O=C(CCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 490.98

Physical Properties

Property code	Value	Unit	Source
gf	-280.12	kJ/mol	Joback Method
hf	-574.01	kJ/mol	Joback Method
hfus	56.29	kJ/mol	Joback Method
hvap	106.58	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.288		Crippen Method
mvol	291.190	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	3470.00		NIST Webbook
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tb	1048.76	K	Joback Method
tc	1301.89	K	Joback Method
tf	733.15	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.22	J/molxK	1048.76	Joback Method
cpg	718.29	J/molxK	1090.95	Joback Method
cpg	722.07	J/molxK	1133.14	Joback Method
cpg	724.57	J/molxK	1175.32	Joback Method
cpg	725.80	J/molxK	1217.51	Joback Method
cpg	725.76	J/molxK	1259.70	Joback Method
cpg	724.48	J/molxK	1301.89	Joback Method
dvisc	0.0001529	Paxs	733.15	Joback Method

dvisc	0.0001118	Paxs	785.75	Joback Method
dvisc	0.0000850	Paxs	838.35	Joback Method
dvisc	0.0000667	Paxs	890.96	Joback Method
dvisc	0.0000538	Paxs	943.56	Joback Method
dvisc	0.0000444	Paxs	996.16	Joback Method
dvisc	0.0000373	Paxs	1048.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359252&Units=SI

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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