Glutaric acid, 2,4,6-trichlorophenyl 3-hexyl ester

Inchi: InChI=1S/C17H21Cl3O4/c1-3-6-12(4-2)23-15(21)7-5-8-16(22)24-17-13(19)9-11(18)10-14

InchiKey: RLMUMLPLPVZKBK-UHFFFAOYSA-N

Formula: C17H21Cl3O4

SMILES: CCCC(CC)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	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	894.41	K	Joback Method
tc	1111.41	K	Joback Method
tf	564.41	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002328	Pa×s	619.41	Joback Method
dvisc	0.0001552	Pa×s	674.41	Joback Method
dvisc	0.0001100	Pa×s	729.41	Joback Method
dvisc	0.0000818	Pa×s	784.41	Joback Method
dvisc	0.0000633	Pa×s	839.41	Joback Method
dvisc	0.0000505	Pa×s	894.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U393561&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