Glutaric acid, isohexyl 2,3,6-trichlorophenyl ester

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

InchiKey: WYMMYIJXBWGCSK-UHFFFAOYSA-N

Formula: C17H21Cl3O4

SMILES: CC(C)CCCOC(=O)CCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl

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	-6.23		Crippen Method
logp	5.702		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		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: 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=U359245&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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