Glutaric acid, 3-methylbut-2-yl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C16H19Cl3O4/c1-9(2)10(3)22-14(20)5-4-6-15(21)23-13-8-11(17)7-12(18)16(13

InchiKey: BYYMVNADMQSYQJ-UHFFFAOYSA-N

Formula: C16H19Cl3O4

SMILES: CC(C)C(C)OC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl

Mol. weight [g/mol]: 381.68

Physical Properties

Property code	Value	Unit	Source
gf	-341.15	kJ/mol	Joback Method
hf	-718.83	kJ/mol	Joback Method
hfus	41.19	kJ/mol	Joback Method
hvap	86.16	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.310		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	871.09	K	Joback Method
tc	1091.17	K	Joback Method
tf	538.14	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.52	J/mol×K	871.09	Joback Method
cpg	769.49	J/mol×K	1054.49	Joback Method
cpg	762.06	J/mol×K	1017.81	Joback Method
cpg	753.55	J/mol×K	981.13	Joback Method
cpg	743.97	J/mol×K	944.45	Joback Method
cpg	733.29	J/mol×K	907.77	Joback Method
cpg	775.86	J/mol×K	1091.17	Joback Method
dvisc	0.0000534	Pa×s	871.09	Joback Method

dvisc	0.0000676	Pa×s	815.60	Joback Method
dvisc	0.0000887	Pa×s	760.11	Joback Method
dvisc	0.0001213	Pa×s	704.62	Joback Method
dvisc	0.0001750	Pa×s	649.12	Joback Method
dvisc	0.0002705	Pa×s	593.63	Joback Method
dvisc	0.0004572	Pa×s	538.14	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=U392176&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