Glutaric acid, isobutyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C15H17Cl3O4/c1-9(2)8-21-13(19)4-3-5-14(20)22-12-7-10(16)6-11(17)15(12)18

InchiKey: OFLLMUNANMNDDH-UHFFFAOYSA-N

Formula: C15H17Cl3O4

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

Mol. weight [g/mol]: 367.65

Physical Properties

Property code	Value	Unit	Source
gf	-347.13	kJ/mol	Joback Method
hf	-692.91	kJ/mol	Joback Method
hfus	42.12	kJ/mol	Joback Method
hvap	84.33	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.922		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2433.00		NIST Webbook
tb	848.65	K	Joback Method
tc	1067.46	K	Joback Method
tf	541.87	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.23	J/mol×K	848.65	Joback Method
cpg	676.64	J/mol×K	885.12	Joback Method
cpg	687.02	J/mol×K	921.59	Joback Method
cpg	696.40	J/mol×K	958.05	Joback Method
cpg	704.76	J/mol×K	994.52	Joback Method
cpg	712.13	J/mol×K	1030.99	Joback Method
cpg	718.50	J/mol×K	1067.46	Joback Method
dvisc	0.0004634	Pa×s	541.87	Joback Method
dvisc	0.0002925	Pa×s	593.00	Joback Method

dvisc	0.0001987	Pa×s	644.13	Joback Method
dvisc	0.0001428	Pa×s	695.26	Joback Method
dvisc	0.0001074	Pa×s	746.39	Joback Method
dvisc	0.0000838	Pa×s	797.52	Joback Method
dvisc	0.0000674	Pa×s	848.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359119&Units=SI
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

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