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

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

InchiKey: ZPTUBGWVTRCLPA-UHFFFAOYSA-N

Formula: C17H21Cl3O4

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

Mol. weight [g/mol]: 395.70

Physical Properties

Property code	Value	Unit	Source
gf	-332.73	kJ/mol	Joback Method
hf	-739.47	kJ/mol	Joback Method
hfus	43.78	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.700		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	893.97	K	Joback Method
tc	1113.16	K	Joback Method
tf	549.41	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.04	J/mol×K	893.97	Joback Method
cpg	826.63	J/mol×K	1076.63	Joback Method
cpg	819.14	J/mol×K	1040.10	Joback Method
cpg	810.55	J/mol×K	1003.56	Joback Method
cpg	800.84	J/mol×K	967.03	Joback Method
cpg	790.01	J/mol×K	930.50	Joback Method
cpg	833.02	J/mol×K	1113.16	Joback Method
dvisc	0.0000461	Pa×s	893.97	Joback Method

dvisc	0.0000586	Pa×s	836.54	Joback Method
dvisc	0.0000772	Pa×s	779.12	Joback Method
dvisc	0.0001061	Pa×s	721.69	Joback Method
dvisc	0.0001541	Pa×s	664.26	Joback Method
dvisc	0.0002402	Pa×s	606.84	Joback Method
dvisc	0.0004110	Pa×s	549.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392177&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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