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

Inchi: InChI=1S/C21H29Cl3O4/c1-3-4-5-6-7-8-10-15(2)27-19(25)11-9-12-20(26)28-18-14-16(22

InchiKey: YKYLONQHIXTJCW-UHFFFAOYSA-N

Formula: C21H29Cl3O4

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

Mol. weight [g/mol]: 451.81

Physical Properties

Property code	Value	Unit	Source
gf	-296.61	kJ/mol	Joback Method
hf	-816.75	kJ/mol	Joback Method
hfus	57.66	kJ/mol	Joback Method
hvap	97.68	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.405		Crippen Method
mcvol	334.590	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook
tb	985.93	K	Joback Method
tc	1208.79	K	Joback Method
tf	609.49	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.56	J/mol×K	985.93	Joback Method
cpg	1023.13	J/mol×K	1023.07	Joback Method
cpg	1034.38	J/mol×K	1060.22	Joback Method
cpg	1044.32	J/mol×K	1097.36	Joback Method
cpg	1052.98	J/mol×K	1134.50	Joback Method
cpg	1060.39	J/mol×K	1171.64	Joback Method
cpg	1066.58	J/mol×K	1208.79	Joback Method
dvisc	0.0002412	Pa×s	609.49	Joback Method

dvisc	0.0001421	Pa×s	672.23	Joback Method
dvisc	0.0000916	Pa×s	734.97	Joback Method
dvisc	0.0000633	Pa×s	797.71	Joback Method
dvisc	0.0000462	Pa×s	860.45	Joback Method
dvisc	0.0000351	Pa×s	923.19	Joback Method
dvisc	0.0000277	Pa×s	985.93	Joback Method

Sources

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=U392186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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