Glutaric acid, 2,3-dichlorophenyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C19H26Cl2O4/c1-13(11-19(2,3)4)12-24-16(22)9-6-10-17(23)25-15-8-5-7-14(20

InchiKey: KSLSXWMJFTYZNL-UHFFFAOYSA-N

Formula: C19H26Cl2O4

SMILES: CC(COC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl)CC(C)(C)C

Mol. weight [g/mol]: 389.31

Physical Properties

Property code	Value	Unit	Source
gf	-289.05	kJ/mol	Joback Method
hf	-757.01	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	86.89	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.685		Crippen Method
mcvol	294.170	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2592.00		NIST Webbook
rinpol	2592.00		NIST Webbook
tb	894.53	K	Joback Method
tc	1111.74	K	Joback Method
tf	546.93	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.75	J/mol×K	894.53	Joback Method
cpg	929.26	J/mol×K	1075.54	Joback Method
cpg	919.88	J/mol×K	1039.34	Joback Method
cpg	909.49	J/mol×K	1003.14	Joback Method
cpg	898.03	J/mol×K	966.93	Joback Method
cpg	885.46	J/mol×K	930.73	Joback Method
cpg	937.67	J/mol×K	1111.74	Joback Method
dvisc	0.0000337	Pa×s	894.53	Joback Method

dvisc	0.0000438	Pa×s	836.60	Joback Method
dvisc	0.0000593	Pa×s	778.66	Joback Method
dvisc	0.0000841	Pa×s	720.73	Joback Method
dvisc	0.0001268	Pa×s	662.80	Joback Method
dvisc	0.0002069	Pa×s	604.86	Joback Method
dvisc	0.0003744	Pa×s	546.93	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=U391539&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