Glutaric acid, 2,4,6-trichlorophenyl phenethyl ester

Inchi: InChI=1S/C19H17Cl3O4/c20-14-11-15(21)19(16(22)12-14)26-18(24)8-4-7-17(23)25-10-9

InchiKey: HREXAOSKQMTJBL-UHFFFAOYSA-N

Formula: C19H17Cl3O4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCCc1ccccc1

Mol. weight [g/mol]: 415.69

Physical Properties

Property code	Value	Unit	Source
gf	-198.60	kJ/mol	Joback Method
hf	-533.66	kJ/mol	Joback Method
hfus	50.05	kJ/mol	Joback Method
hvap	95.89	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.508		Crippen Method
mcvol	282.650	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2947.00		NIST Webbook
rinpol	2947.00		NIST Webbook
tb	967.29	K	Joback Method
tc	1204.77	K	Joback Method
tf	628.37	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.07	J/mol×K	967.29	Joback Method
cpg	794.84	J/mol×K	1006.87	Joback Method
cpg	803.35	J/mol×K	1046.45	Joback Method
cpg	810.65	J/mol×K	1086.03	Joback Method
cpg	816.76	J/mol×K	1125.61	Joback Method
cpg	821.73	J/mol×K	1165.19	Joback Method
cpg	825.57	J/mol×K	1204.77	Joback Method
dvisc	0.0002633	Pa×s	628.37	Joback Method

dvisc	0.0001716	Pa×s	684.86	Joback Method
dvisc	0.0001193	Pa×s	741.34	Joback Method
dvisc	0.0000874	Pa×s	797.83	Joback Method
dvisc	0.0000667	Pa×s	854.32	Joback Method
dvisc	0.0000526	Pa×s	910.80	Joback Method
dvisc	0.0000427	Pa×s	967.29	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=U391798&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