Glutaric acid, 2-(adamant-1-yl)ethyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C19H28Cl2O4/c20-16(21)12-25-18(23)3-1-2-17(22)24-5-4-19-9-13-6-14(10-19
InchiKey: FYIOEDIEEKKGJP-UHFFFAOYSA-N
Formula: C19H28Cl2O4
SMILES: O=C(CCCC(=O)OCC(Cl)Cl)OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 391.33

Physical Properties

Property code	Value	Unit	Source
gf	-228.09	kJ/mol	Joback Method
hf	-754.71	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.653		Crippen Method
mcvol	285.350	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	881.18	K	Joback Method
tc	1098.60	K	Joback Method
tf	563.01	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.53	J/mol×K	881.18	Joback Method
cpg	944.43	J/mol×K	917.42	Joback Method
cpg	963.03	J/mol×K	953.65	Joback Method
cpg	981.50	J/mol×K	989.89	Joback Method
cpg	1000.03	J/mol×K	1026.13	Joback Method
cpg	1018.80	J/mol×K	1062.36	Joback Method
cpg	1038.00	J/mol×K	1098.60	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=U405380&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
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