Glutaric acid, tridec-2-yn-1-yl 2,2-dichloroethyl ester

Inchi: InChI=1S/C20H32Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-25-19(23)14-13-15-20(24)26-17
InchiKey: JUMAKTXMLFVCGA-UHFFFAOYSA-N
Formula: C20H32Cl2O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 407.37

Physical Properties

Property code	Value	Unit	Source
gf	-173.82	kJ/mol	Joback Method
hf	-710.19	kJ/mol	Joback Method
hfus	61.12	kJ/mol	Joback Method
hvap	88.96	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.581		Crippen Method
mcvol	323.420	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2727.00		NIST Webbook
rinpol	2727.00		NIST Webbook
tb	893.00	K	Joback Method
tc	1097.03	K	Joback Method
tf	610.42	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.64	J/mol×K	893.00	Joback Method
cpg	992.99	J/mol×K	927.00	Joback Method
cpg	1007.21	J/mol×K	961.01	Joback Method
cpg	1020.31	J/mol×K	995.01	Joback Method
cpg	1032.33	J/mol×K	1029.02	Joback Method
cpg	1043.28	J/mol×K	1063.02	Joback Method
cpg	1053.18	J/mol×K	1097.03	Joback Method

Sources

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=U393543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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