Glutaric acid, 2,2-dichloroethyl non-5-yn-3-yl ester

Inchi: InChI=1S/C16H24Cl2O4/c1-3-5-6-7-9-13(4-2)22-16(20)11-8-10-15(19)21-12-14(17)18/h1

InchiKey: BYVUKBFXOUCSNP-UHFFFAOYSA-N

Formula: C16H24Cl2O4

SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 351.26

Physical Properties

Property code	Value	Unit	Source
gf	-209.94	kJ/mol	Joback Method
hf	-632.91	kJ/mol	Joback Method
hfus	47.24	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.019		Crippen Method
mcvol	267.060	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	801.04	K	Joback Method
tc	1003.32	K	Joback Method
tf	550.34	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.40	J/mol×K	801.04	Joback Method
cpg	759.74	J/mol×K	834.75	Joback Method
cpg	773.12	J/mol×K	868.47	Joback Method
cpg	785.55	J/mol×K	902.18	Joback Method
cpg	797.03	J/mol×K	935.89	Joback Method
cpg	807.59	J/mol×K	969.60	Joback Method
cpg	817.23	J/mol×K	1003.32	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=U393954&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