Glutaric acid, dodec-9-ynyl propyl ester

Inchi: InChI=1S/C20H34O4/c1-3-5-6-7-8-9-10-11-12-13-18-24-20(22)16-14-15-19(21)23-17-4-2
InchiKey: QSAICPKQMDGYFR-UHFFFAOYSA-N
Formula: C20H34O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCCC
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-147.52	kJ/mol	Joback Method
hf	-673.43	kJ/mol	Joback Method
hfus	56.25	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.797		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1200.62	kPa	Joback Method
rinpol	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook
tb	818.58	K	Joback Method
tc	1009.33	K	Joback Method
tf	565.58	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.80	J/mol×K	818.58	Joback Method
cpg	937.14	J/mol×K	850.37	Joback Method
cpg	953.44	J/mol×K	882.16	Joback Method
cpg	968.72	J/mol×K	913.95	Joback Method
cpg	982.99	J/mol×K	945.75	Joback Method
cpg	996.27	J/mol×K	977.54	Joback Method
cpg	1008.57	J/mol×K	1009.33	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=U359784&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

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