

Glutaric acid, dodec-9-ynyl hexyl ester

Inchi: InChI=1S/C23H40O4/c1-3-5-7-9-10-11-12-13-14-16-21-27-23(25)19-17-18-22(24)26-20-
InchiKey: WRTJUVHERGRWMG-UHFFFAOYSA-N
Formula: C23H40O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-122.26	kJ/mol	Joback Method
hf	-735.35	kJ/mol	Joback Method
hfus	64.02	kJ/mol	Joback Method
hvap	87.26	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.967		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	992.63	kPa	Joback Method
rinpol	2751.00		NIST Webbook
rinpol	2751.00		NIST Webbook
tb	887.22	K	Joback Method
tc	1086.71	K	Joback Method
tf	599.39	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.54	J/mol×K	887.22	Joback Method
cpg	1120.90	J/mol×K	920.47	Joback Method
cpg	1138.02	J/mol×K	953.72	Joback Method
cpg	1153.93	J/mol×K	986.96	Joback Method
cpg	1168.64	J/mol×K	1020.21	Joback Method
cpg	1182.19	J/mol×K	1053.46	Joback Method
cpg	1194.59	J/mol×K	1086.71	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=U359789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvac:	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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