

Glutaric acid, but-3-yn-2-yl pentadecyl ester

Inchi: InChI=1S/C24H42O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-21-27-23(25)19-18-20-24(2)
InchiKey: FLQMUBQZMHUAIZ-UHFFFAOYSA-N
Formula: C24H42O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-96.01	kJ/mol	Joback Method
hf	-741.67	kJ/mol	Joback Method
hfus	62.94	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.356		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	932.92	kPa	Joback Method
rinpola	2722.00		NIST Webbook
tb	890.78	K	Joback Method
tc	1090.57	K	Joback Method
tf	536.53	K	Joback Method
vc	1.383	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.20	J/mol×K	890.78	Joback Method
cpg	1177.05	J/mol×K	924.08	Joback Method
cpg	1194.65	J/mol×K	957.38	Joback Method
cpg	1211.03	J/mol×K	990.68	Joback Method
cpg	1226.24	J/mol×K	1023.97	Joback Method
cpg	1240.29	J/mol×K	1057.27	Joback Method
cpg	1253.24	J/mol×K	1090.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U359886&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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