

Glutaric acid, non-5-yn-3-yl tridecyl ester

Inchi: InChI=1S/C27H48O4/c1-4-7-9-11-12-13-14-15-16-17-19-24-30-26(28)22-20-23-27(29)31
InchiKey: NEIUIKPLIAPDDE-UHFFFAOYSA-N
Formula: C27H48O4
SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-91.02	kJ/mol	Joback Method
hf	-823.19	kJ/mol	Joback Method
hfus	70.86	kJ/mol	Joback Method
hvap	95.77	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.526		Crippen Method
mvol	397.570	ml/mol	McGowan Method
pc	793.49	kPa	Joback Method
rinpol	3022.00		NIST Webbook
tb	978.30	K	Joback Method
tc	1201.23	K	Joback Method
tf	629.47	K	Joback Method
vc	1.552	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1354.91	J/mol×K	978.30	Joback Method
cpg	1374.81	J/mol×K	1015.46	Joback Method
cpg	1393.05	J/mol×K	1052.61	Joback Method
cpg	1409.66	J/mol×K	1089.77	Joback Method
cpg	1424.69	J/mol×K	1126.92	Joback Method
cpg	1438.20	J/mol×K	1164.08	Joback Method
cpg	1450.23	J/mol×K	1201.23	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=U359810&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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