Glutaric acid, hex-4-yn-3-yl pentadecyl ester

Inchi: InChI=1S/C26H46O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-23-29-25(27)21-19-22-26(
InchiKey: ACZVFNOVJGRLOD-UHFFFAOYSA-N
Formula: C26H46O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-99.44	kJ/mol	Joback Method
hf	-802.55	kJ/mol	Joback Method
hfus	68.27	kJ/mol	Joback Method
hvap	93.55	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.136		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	838.21	kPa	Joback Method
rinpol	2962.00		NIST Webbook
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tb	955.42	K	Joback Method
tc	1170.99	K	Joback Method
tf	618.20	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.21	J/mol×K	955.42	Joback Method
cpg	1310.69	J/mol×K	991.35	Joback Method
cpg	1328.62	J/mol×K	1027.28	Joback Method
cpg	1345.05	J/mol×K	1063.21	Joback Method
cpg	1360.01	J/mol×K	1099.13	Joback Method
cpg	1373.54	J/mol×K	1135.06	Joback Method
cpg	1385.70	J/mol×K	1170.99	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=U359866&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