Glutaric acid, hex-4-yn-3-yl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C23H36O4/c1-4-7-8-9-10-11-12-13-14-15-20-26-22(24)18-16-19-23(25)27-21(

InchiKey: YVIFVYSKJCDDSC-UHFFFAOYSA-N

Formula: C23H36O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCCCCC#CCC

Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	78.10	kJ/mol	Joback Method
hf	-468.33	kJ/mol	Joback Method
hfus	63.62	kJ/mol	Joback Method
hvap	89.02	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	5.189		Crippen Method
mcvol	332.610	ml/mol	McGowan Method
pc	1106.68	kPa	Joback Method
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook
tb	895.78	K	Joback Method
tc	1101.62	K	Joback Method
tf	690.49	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.28	J/mol×K	895.78	Joback Method
cpg	1067.66	J/mol×K	930.09	Joback Method
cpg	1083.80	J/mol×K	964.39	Joback Method
cpg	1098.71	J/mol×K	998.70	Joback Method
cpg	1112.42	J/mol×K	1033.01	Joback Method
cpg	1124.96	J/mol×K	1067.32	Joback Method
cpg	1136.33	J/mol×K	1101.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393943&Units=SI
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

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