Glutaric acid, hexyl tridec-2-ynyl ester

Inchi: InChI=1S/C24H42O4/c1-3-5-7-9-10-11-12-13-14-15-17-22-28-24(26)20-18-19-23(25)27-
InchiKey: ZILRHCLOCARFBA-UHFFFAOYSA-N
Formula: C24H42O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCCCCCC
Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-113.84	kJ/mol	Joback Method
hf	-755.99	kJ/mol	Joback Method
hfus	66.61	kJ/mol	Joback Method
hvap	89.48	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.358		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	935.20	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	910.10	K	Joback Method
tc	1114.22	K	Joback Method
tf	610.66	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.77	J/mol×K	910.10	Joback Method
cpg	1183.51	J/mol×K	944.12	Joback Method
cpg	1200.93	J/mol×K	978.14	Joback Method
cpg	1217.04	J/mol×K	1012.16	Joback Method
cpg	1231.88	J/mol×K	1046.18	Joback Method
cpg	1245.49	J/mol×K	1080.20	Joback Method
cpg	1257.88	J/mol×K	1114.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360125&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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