Glutaric acid, propyl tridec-2-ynyl ester

Inchi: InChI=1S/C21H36O4/c1-3-5-6-7-8-9-10-11-12-13-14-19-25-21(23)17-15-16-20(22)24-18
InchiKey: YCMJGOCMZCRMAY-UHFFFAOYSA-N
Formula: C21H36O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-139.10	kJ/mol	Joback Method
hf	-694.07	kJ/mol	Joback Method
hfus	58.84	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.187		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1124.57	kPa	Joback Method
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
tb	841.46	K	Joback Method
tc	1034.33	K	Joback Method
tf	576.85	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.99	J/mol×K	841.46	Joback Method
cpg	997.66	J/mol×K	873.60	Joback Method
cpg	1014.23	J/mol×K	905.75	Joback Method
cpg	1029.72	J/mol×K	937.89	Joback Method
cpg	1044.15	J/mol×K	970.04	Joback Method
cpg	1057.53	J/mol×K	1002.18	Joback Method
cpg	1069.89	J/mol×K	1034.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360120&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

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