Glutaric acid, heptyl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C21H36O4/c1-5-7-9-10-11-16-24-20(22)14-12-15-21(23)25-19(13-8-6-2)17-18

InchiKey: APVBEXAVCUMEJR-UHFFFAOYSA-N

Formula: C21H36O4

SMILES: CCC#CC(CC(C)C)OC(=O)CCCC(=O)OCCCCCCC

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-143.98	kJ/mol	Joback Method
hf	-704.63	kJ/mol	Joback Method
hfus	51.80	kJ/mol	Joback Method
hvap	82.03	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.042		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	3464.00		NIST Webbook
tb	840.58	K	Joback Method
tc	1035.64	K	Joback Method
tf	546.85	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.96	J/mol×K	840.58	Joback Method
cpg	998.81	J/mol×K	873.09	Joback Method
cpg	1015.52	J/mol×K	905.60	Joback Method
cpg	1031.10	J/mol×K	938.11	Joback Method
cpg	1045.58	J/mol×K	970.62	Joback Method
cpg	1058.97	J/mol×K	1003.13	Joback Method
cpg	1071.30	J/mol×K	1035.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359604&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