

Glutaric acid, heptyl non-5-yn-3-yl ester

Inchi:	InChI=1S/C21H36O4/c1-4-7-9-11-13-18-24-20(22)16-14-17-21(23)25-19(6-3)15-12-10-8
InchiKey:	UKMLZDSHEONLQS-UHFFFAOYSA-N
Formula:	C21H36O4
SMILES:	CCCC#CCC(CC)OC(=O)CCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	352.51

Physical Properties

Property code	Value	Unit	Source
gf	-141.54	kJ/mol	Joback Method
hf	-699.35	kJ/mol	Joback Method
hfus	55.32	kJ/mol	Joback Method
hvap	82.42	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.186		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinqol	2411.00		NIST Webbook
tb	841.02	K	Joback Method
tc	1034.92	K	Joback Method
tf	561.85	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.47	J/molxK	841.02	Joback Method
cpg	998.23	J/molxK	873.34	Joback Method
cpg	1014.86	J/molxK	905.65	Joback Method
cpg	1030.39	J/molxK	937.97	Joback Method
cpg	1044.85	J/molxK	970.28	Joback Method
cpg	1058.23	J/molxK	1002.60	Joback Method
cpg	1070.57	J/molxK	1034.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359804&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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