

Glutaric acid, 2,7-dimethyloct-5-yn-7-en-4-yl heptyl ester

Inchi:	InChI=1S/C22H36O4/c1-6-7-8-9-10-16-25-21(23)12-11-13-22(24)26-20(17-19(4)5)15-14
InchiKey:	ITEUKWQQCAGRRG-UHFFFAOYSA-N
Formula:	C22H36O4
SMILES:	<chem>C=C(C)C#CC(CC(C)C)OC(=O)CCCC(=O)OCCCCCCC</chem>
Mol. weight [g/mol]:	364.52

Physical Properties

Property code	Value	Unit	Source
gf	-56.27	kJ/mol	Joback Method
hf	-609.63	kJ/mol	Joback Method
hfus	51.80	kJ/mol	Joback Method
hvap	83.66	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.208		Crippen Method
mvol	322.820	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
tb	860.02	K	Joback Method
tc	1058.85	K	Joback Method
tf	542.40	K	Joback Method
vc	1.248	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.51	J/mol×K	860.02	Joback Method
cpg	1031.22	J/mol×K	893.16	Joback Method
cpg	1047.78	J/mol×K	926.30	Joback Method
cpg	1063.19	J/mol×K	959.43	Joback Method
cpg	1077.49	J/mol×K	992.57	Joback Method
cpg	1090.69	J/mol×K	1025.71	Joback Method
cpg	1102.84	J/mol×K	1058.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U359841&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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