Glutaric acid, 2,6-dimethylnon-1-en-3-yn-5-yl pentyl ester

Inchi: InChI=1S/C21H34O4/c1-6-8-9-16-24-20(22)12-10-13-21(23)25-19(15-14-17(3)4)18(5)11

InchiKey: TVMBAHYGEUTBBL-UHFFFAOYSA-N

Formula: C21H34O4

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

Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-64.69	kJ/mol	Joback Method
hf	-588.99	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.818		Crippen Method
mcvol	308.730	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2256.00		NIST Webbook
tb	837.14	K	Joback Method
tc	1034.39	K	Joback Method
tf	531.13	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.10	J/mol×K	837.14	Joback Method
cpg	970.57	J/mol×K	870.02	Joback Method
cpg	986.93	J/mol×K	902.89	Joback Method
cpg	1002.19	J/mol×K	935.77	Joback Method
cpg	1016.39	J/mol×K	968.64	Joback Method
cpg	1029.53	J/mol×K	1001.52	Joback Method
cpg	1041.66	J/mol×K	1034.39	Joback Method

Sources

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=U359821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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