

Glutaric acid, tridec-2-yn-1-yl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C26H46O4/c1-6-7-8-9-10-11-12-13-14-15-16-20-29-24(27)18-17-19-25(28)30-
InchiKey: JHYLAFDVGIIIDY-UHFFFAOYSA-N
Formula: C26H46O4
SMILES: CCCCCCCCCC#CCOC(=O)CCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-96.60	kJ/mol	Joback Method
hf	-811.30	kJ/mol	Joback Method
hfus	60.85	kJ/mol	Joback Method
hvap	92.25	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.850		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	847.51	kPa	Joback Method
rinpol	2835.00		NIST Webbook
rinpol	2835.00		NIST Webbook
tb	952.19	K	Joback Method
tc	1165.84	K	Joback Method
tf	620.62	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.04	J/mol×K	952.19	Joback Method
cpg	1310.33	J/mol×K	987.80	Joback Method
cpg	1328.21	J/mol×K	1023.41	Joback Method
cpg	1344.72	J/mol×K	1059.02	Joback Method
cpg	1359.93	J/mol×K	1094.63	Joback Method
cpg	1373.91	J/mol×K	1130.23	Joback Method
cpg	1386.70	J/mol×K	1165.84	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=U391543&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
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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