

Glutaric acid, 3-methylbut-2-yl dodec-9-yn-1-yl ester

Inchi:	InChI=1S/C22H38O4/c1-5-6-7-8-9-10-11-12-13-14-18-25-21(23)16-15-17-22(24)26-20(4
InchiKey:	AZRYTSKRSDZAJQ-UHFFFAOYSA-N
Formula:	C22H38O4
SMILES:	CCC#CCCCCCCCOC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	366.53

Physical Properties

Property code	Value	Unit	Source
gf	-135.56	kJ/mol	Joback Method
hf	-725.27	kJ/mol	Joback Method
hfus	54.39	kJ/mol	Joback Method
hvap	84.25	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.432		Crippen Method
mvol	327.120	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	863.46	K	Joback Method
tc	1060.75	K	Joback Method
tf	558.12	K	Joback Method
vc	1.266	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.86	J/molxK	863.46	Joback Method
cpg	1059.98	J/molxK	896.34	Joback Method
cpg	1076.90	J/molxK	929.22	Joback Method
cpg	1092.63	J/molxK	962.11	Joback Method
cpg	1107.20	J/molxK	994.99	Joback Method
cpg	1120.63	J/molxK	1027.87	Joback Method
cpg	1132.95	J/molxK	1060.75	Joback Method

Sources

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=U393940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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