Glutaric acid, tridec-2-yn-1-yl 3-methylbut-2-yl ester

Inchi: InChI=1S/C23H40O4/c1-5-6-7-8-9-10-11-12-13-14-15-19-26-22(24)17-16-18-23(25)27-2
InchiKey: ITTRJWLKFIPLRK-UHFFFAOYSA-N
Formula: C23H40O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-127.14	kJ/mol	Joback Method
hf	-745.91	kJ/mol	Joback Method
hfus	56.98	kJ/mol	Joback Method
hvap	86.48	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.822		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinpol	2577.00		NIST Webbook
rinpol	2577.00		NIST Webbook
tb	886.34	K	Joback Method
tc	1086.67	K	Joback Method
tf	569.39	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.44	J/mol×K	886.34	Joback Method
cpg	1121.84	J/mol×K	919.73	Joback Method
cpg	1138.97	J/mol×K	953.12	Joback Method
cpg	1154.84	J/mol×K	986.50	Joback Method
cpg	1169.50	J/mol×K	1019.89	Joback Method
cpg	1182.95	J/mol×K	1053.28	Joback Method
cpg	1195.24	J/mol×K	1086.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393575&Units=SI
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

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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