

Succinic acid, tridec-2-yn-1-yl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C23H40O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-26-21(24)17-18-22(25)27-20(21)
InchiKey: ZVLHBJJTTLNMRA-UHFFFAOYSA-N
Formula: C23H40O4
SMILES: CCCCCCCCCC#CCOC(=O)CCC(=O)OC(C)C(C)C(C)C
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-121.86	kJ/mol	Joback Method
hf	-749.38	kJ/mol	Joback Method
hfus	53.09	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.822		Crippen Method
mvol	341.210	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	883.55	K	Joback Method
tc	1084.84	K	Joback Method
tf	586.81	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.33	J/mol×K	883.55	Joback Method
cpg	1121.67	J/mol×K	917.10	Joback Method
cpg	1138.78	J/mol×K	950.65	Joback Method
cpg	1154.73	J/mol×K	984.19	Joback Method
cpg	1169.53	J/mol×K	1017.74	Joback Method
cpg	1183.25	J/mol×K	1051.29	Joback Method
cpg	1195.91	J/mol×K	1084.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U390635&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
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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