Sebacic acid, isobutyl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C23H40O4/c1-6-7-14-21(17-19(2)3)27-23(25)16-13-11-9-8-10-12-15-22(24)26

InchiKey: FTJFBSKXDUBRQU-UHFFFAOYSA-N

Formula: C23H40O4

SMILES: CCC#CC(CC(C)C)OC(=O)CCCCCCCCC(=O)OCC(C)C

Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-129.58	kJ/mol	Joback Method
hf	-751.19	kJ/mol	Joback Method
hfus	53.45	kJ/mol	Joback Method
hvap	86.09	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.678		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	1007.81	kPa	Joback Method
rinpol	2472.00		NIST Webbook
rinpol	2472.00		NIST Webbook
tb	885.90	K	Joback Method
tc	1086.86	K	Joback Method
tf	554.39	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.90	J/mol×K	885.90	Joback Method
cpg	1122.33	J/mol×K	919.39	Joback Method
cpg	1139.47	J/mol×K	952.89	Joback Method
cpg	1155.35	J/mol×K	986.38	Joback Method
cpg	1169.99	J/mol×K	1019.87	Joback Method
cpg	1183.41	J/mol×K	1053.37	Joback Method
cpg	1195.64	J/mol×K	1086.86	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=U355868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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