Sebacic acid, 2,6-dimethylnon-1-en-3-yn-5-yl isobutyl ester

Inchi: InChI=1S/C25H42O4/c1-7-14-22(6)23(18-17-20(2)3)29-25(27)16-13-11-9-8-10-12-15-24

InchiKey: SFXYSQLVMVLFIT-UHFFFAOYSA-N

Formula: C25H42O4

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

Mol. weight [g/mol]: 406.60

Physical Properties

Property code	Value	Unit	Source
gf	-33.45	kJ/mol	Joback Method
hf	-676.83	kJ/mol	Joback Method
hfus	56.04	kJ/mol	Joback Method
hvap	89.95	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.234		Crippen Method
mcvol	365.090	ml/mol	McGowan Method
pc	921.06	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	928.22	K	Joback Method
tc	1136.87	K	Joback Method
tf	561.21	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.11	J/mol×K	928.22	Joback Method
cpg	1217.65	J/mol×K	962.99	Joback Method
cpg	1234.80	J/mol×K	997.77	Joback Method
cpg	1250.61	J/mol×K	1032.54	Joback Method
cpg	1265.12	J/mol×K	1067.32	Joback Method
cpg	1278.36	J/mol×K	1102.09	Joback Method
cpg	1290.38	J/mol×K	1136.87	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=U355805&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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