

Sebacic acid, 2,7-dimethylocta-7-en-5-yn-4-yl isobutyl ester

Inchi: InChI=1S/C24H40O4/c1-19(2)15-16-22(17-20(3)4)28-24(26)14-12-10-8-7-9-11-13-23(25)
InchiKey: DRVBDKSCCHKMLN-UHFFFAOYSA-N
Formula: C24H40O4
SMILES: C=C(C)C#CC(CC(C)C)OC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-41.87	kJ/mol	Joback Method
hf	-656.19	kJ/mol	Joback Method
hfus	53.45	kJ/mol	Joback Method
hvap	87.73	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.844		Crippen Method
mcvol	351.000	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	2507.00		NIST Webbook
tb	905.34	K	Joback Method
tc	1110.27	K	Joback Method
tf	549.94	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.81	J/molxK	905.34	Joback Method
cpg	1155.08	J/molxK	939.50	Joback Method
cpg	1172.05	J/molxK	973.65	Joback Method
cpg	1187.74	J/molxK	1007.81	Joback Method
cpg	1202.19	J/molxK	1041.96	Joback Method
cpg	1215.43	J/molxK	1076.12	Joback Method
cpg	1227.50	J/molxK	1110.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U355814&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
hvac:	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

Latest version available from:

<https://www.chemeo.com/cid/48-628-2/Sebacic-acid-2-7-dimethylocta-7-en-5-yn-4-yl-isobutyl-ester.pdf>

Generated by Cheméo on 2024-04-29 15:04:17.76589198 +0000 UTC m=+16692306.686469293.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.