

Sebacic acid, isohexyl non-5-yn-3-yl ester

Inchi: InChI=1S/C25H44O4/c1-5-7-8-13-18-23(6-2)29-25(27)20-15-12-10-9-11-14-19-24(26)28
InchiKey: SCAKKVPIUAWGRZ-UHFFFAOYSA-N
Formula: C25H44O4
SMILES: CCCC#CCC(CC)OC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-110.30	kJ/mol	Joback Method
hf	-787.19	kJ/mol	Joback Method
hfus	62.16	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.602		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	891.07	kPa	Joback Method
rinpola	2743.00		NIST Webbook
rinpola	2743.00		NIST Webbook
tb	932.10	K	Joback Method
tc	1141.17	K	Joback Method
tf	591.93	K	Joback Method
vc	1.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1228.36	J/molxK	932.10	Joback Method
cpg	1247.39	J/molxK	966.95	Joback Method
cpg	1264.96	J/molxK	1001.79	Joback Method
cpg	1281.13	J/molxK	1036.64	Joback Method
cpg	1295.93	J/molxK	1071.48	Joback Method
cpg	1309.38	J/molxK	1106.33	Joback Method
cpg	1321.53	J/molxK	1141.17	Joback Method

Sources

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=U355801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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