

Sebacic acid, heptyl hex-4-yn-3-yl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C23H40O4/c1-4-7-8-13-16-20-26-22(24)18-14-11-9-10-12-15-19-23(25)27-21(26)

DRIWMITZMYMGAW-UHFFFAOYSA-N

C23H40O4

CC#CC(CC)OC(=O)CCCCCCCCC(=O)OCCCCCCC

380.56

Physical Properties

Property code	Value	Unit	Source
gf	-124.70	kJ/mol	Joback Method
hf	-740.63	kJ/mol	Joback Method
hfus	60.50	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.966		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	2628.00		NIST Webbook
tb	886.78	K	Joback Method
tc	1086.62	K	Joback Method
tf	584.39	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.99	J/mol×K	886.78	Joback Method
cpg	1121.36	J/mol×K	920.09	Joback Method
cpg	1138.48	J/mol×K	953.39	Joback Method
cpg	1154.37	J/mol×K	986.70	Joback Method
cpg	1169.05	J/mol×K	1020.00	Joback Method
cpg	1182.55	J/mol×K	1053.31	Joback Method
cpg	1194.89	J/mol×K	1086.62	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=U355824&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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