

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

Inchi:	InChI=1S/C28H50O4/c1-5-7-9-10-13-16-19-23-31-27(29)21-17-14-11-12-15-18-22-28(30)
InchiKey:	SRIULFXPAMRLRM-UHFFFAOYSA-N
Formula:	C28H50O4
SMILES:	CCC#CC(CC(C)C)OC(=O)CCCCCCCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	450.69

Physical Properties

Property code	Value	Unit	Source
gf	-85.04	kJ/mol	Joback Method
hf	-849.11	kJ/mol	Joback Method
hfus	69.93	kJ/mol	Joback Method
hvap	97.61	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.772		Crippen Method
mcvol	411.660	ml/mol	McGowan Method
pc	755.57	kPa	Joback Method
rinpol	2999.00		NIST Webbook
tb	1000.74	K	Joback Method
tc	1230.70	K	Joback Method
tf	625.74	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1419.28	J/mol×K	1000.74	Joback Method
cpg	1439.46	J/mol×K	1039.07	Joback Method
cpg	1457.84	J/mol×K	1077.39	Joback Method
cpg	1474.46	J/mol×K	1115.72	Joback Method
cpg	1489.39	J/mol×K	1154.05	Joback Method
cpg	1502.67	J/mol×K	1192.37	Joback Method
cpg	1514.38	J/mol×K	1230.70	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=U355873&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

Latest version available from:

<https://www.chemeo.com/cid/33-144-5/Sebacic-acid-2-methyloct-5-yn-4-yl-nonyl-ester.pdf>

Generated by Cheméo on 2025-12-05 19:37:05.82235474 +0000 UTC m=+4711623.352395406.

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