

Succinic acid, hex-4-yn-3-yl tetradec-3-en-1-yl ester

Inchi:	InChI=1S/C24H40O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-21-27-23(25)19-20-24(26)28-
InchiKey:	VNXQQQBEMCSBIK-FOCLMDBBSA-N
Formula:	C24H40O4
SMILES:	CC#CC(CC)OC(=O)CCC(=O)OCCC=CCCCCCCCCCC
Mol. weight [g/mol]:	392.57

Physical Properties

Property code	Value	Unit	Source
gf	-36.06	kJ/mol	Joback Method
hf	-644.05	kJ/mol	Joback Method
hfus	63.29	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.132		Crippen Method
mvol	351.000	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	913.82	K	Joback Method
tc	1119.31	K	Joback Method
tf	590.58	K	Joback Method
vc	1.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.85	J/molxK	913.82	Joback Method
cpg	1156.08	J/molxK	948.07	Joback Method
cpg	1173.08	J/molxK	982.32	Joback Method
cpg	1188.88	J/molxK	1016.56	Joback Method
cpg	1203.53	J/molxK	1050.81	Joback Method
cpg	1217.08	J/molxK	1085.06	Joback Method
cpg	1229.55	J/molxK	1119.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391056&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	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.cheméo.com/cid/84-133-1/Succinic-acid-hex-4-yn-3-yl-tetradec-3-en-1-yl-ester.pdf>

Generated by Cheméo on 2024-04-28 19:50:01.217306051 +0000 UTC m=+16623050.137883373.

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