

Succinic acid, tridec-2-yn-1-yl 2-ethylbutyl ester

Inchi:	InChI=1S/C23H40O4/c1-4-7-8-9-10-11-12-13-14-15-16-19-26-22(24)17-18-23(25)27-20-
InchiKey:	MFPWSYUCAWCDAX-UHFFFAOYSA-N
Formula:	C23H40O4
SMILES:	CCCCCCCCCCC#CCOC(=O)CCC(=O)OCC(CC)CC
Mol. weight [g/mol]:	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	-6.73		Crippen Method
logp	5.823		Crippen Method
mvol	341.210	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	2683.00		NIST Webbook
rinpol	2683.00		NIST Webbook
tb	886.78	K	Joback Method
tc	1086.62	K	Joback Method
tf	584.39	K	Joback Method
vc	1.327	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389621&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
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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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