

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

Inchi:	InChI=1S/C22H38O4/c1-4-6-7-8-9-10-11-12-13-14-15-18-25-21(23)16-17-22(24)26-19-2
InchiKey:	NWGWTWCOUPVMRD-UHFFFAOYSA-N
Formula:	C22H38O4
SMILES:	CCCCCCCCCCC#CCOC(=O)CCC(=O)OCC(C)CC
Mol. weight [g/mol]:	366.53

Physical Properties

Property code	Value	Unit	Source
gf	-133.12	kJ/mol	Joback Method
hf	-719.99	kJ/mol	Joback Method
hfus	57.91	kJ/mol	Joback Method
hvap	84.64	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.433		Crippen Method
mvol	327.120	ml/mol	McGowan Method
pc	1061.02	kPa	Joback Method
rinpol	2588.00		NIST Webbook
rinpol	2588.00		NIST Webbook
tb	863.90	K	Joback Method
tc	1060.36	K	Joback Method
tf	573.12	K	Joback Method
vc	1.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.39	J/molxK	863.90	Joback Method
cpg	1059.45	J/molxK	896.64	Joback Method
cpg	1076.32	J/molxK	929.39	Joback Method
cpg	1092.03	J/molxK	962.13	Joback Method
cpg	1106.60	J/molxK	994.87	Joback Method
cpg	1120.05	J/molxK	1027.61	Joback Method
cpg	1132.41	J/molxK	1060.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U389641&Units=SI

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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