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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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