Succinic acid, tridec-2-yn-1-yl 4-octyl ester

Inchi: InChI=1S/C25H44O4/c1-4-7-9-10-11-12-13-14-15-16-17-22-28-24(26)20-21-25(27)29-23
InchiKey: MAUTVIBFWJDODB-UHFFFAOYSA-N
Formula: C25H44O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OC(CCC)CCCC
Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-107.86	kJ/mol	Joback Method
hf	-781.91	kJ/mol	Joback Method
hfus	65.68	kJ/mol	Joback Method
hvap	91.32	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.746		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	886.83	kPa	Joback Method
rinpol	2771.00		NIST Webbook
rinpol	2771.00		NIST Webbook
tb	932.54	K	Joback Method
tc	1141.86	K	Joback Method
tf	606.93	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1227.96	J/mol×K	932.54	Joback Method
cpg	1247.04	J/mol×K	967.43	Joback Method
cpg	1264.68	J/mol×K	1002.31	Joback Method
cpg	1280.93	J/mol×K	1037.20	Joback Method
cpg	1295.80	J/mol×K	1072.09	Joback Method
cpg	1309.35	J/mol×K	1106.98	Joback Method
cpg	1321.59	J/mol×K	1141.86	Joback Method

Sources

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=U389572&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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