Succinic acid, tridec-2-yn-1-yl 3-heptyl ester

Inchi: InChI=1S/C24H42O4/c1-4-7-9-10-11-12-13-14-15-16-17-21-27-23(25)19-20-24(26)28-22
InchiKey: ZCWBNJFNEHESFZ-UHFFFAOYSA-N
Formula: C24H42O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OC(CC)CCCC
Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-116.28	kJ/mol	Joback Method
hf	-761.27	kJ/mol	Joback Method
hfus	63.09	kJ/mol	Joback Method
hvap	89.09	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.356		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	939.79	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	909.66	K	Joback Method
tc	1113.76	K	Joback Method
tf	595.66	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.20	J/mol×K	909.66	Joback Method
cpg	1183.91	J/mol×K	943.68	Joback Method
cpg	1201.29	J/mol×K	977.69	Joback Method
cpg	1217.35	J/mol×K	1011.71	Joback Method
cpg	1232.13	J/mol×K	1045.73	Joback Method
cpg	1245.66	J/mol×K	1079.74	Joback Method
cpg	1257.97	J/mol×K	1113.76	Joback Method

Sources

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=U390612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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