Succinic acid, hex-4-yn-3-yl tetrahydrofurfuryl ester

Inchi: InChI=1S/C15H22O5/c1-3-6-12(4-2)20-15(17)9-8-14(16)19-11-13-7-5-10-18-13/h12-13H

InchiKey: YGWUERSTLJGXMJ-UHFFFAOYSA-N

Formula: C15H22O5

SMILES: CC#CC(CC)OC(=O)CCC(=O)OCC1CCCO1

Mol. weight [g/mol]: 282.33

Physical Properties

Property code	Value	Unit	Source
gf	-241.63	kJ/mol	Joback Method
hf	-647.03	kJ/mol	Joback Method
hfus	41.69	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.834		Crippen Method
mcvol	223.500	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	2039.00		NIST Webbook
tb	745.97	K	Joback Method
tc	958.69	K	Joback Method
tf	531.70	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.30	J/mol×K	745.97	Joback Method
cpg	672.80	J/mol×K	781.42	Joback Method
cpg	688.19	J/mol×K	816.88	Joback Method
cpg	702.48	J/mol×K	852.33	Joback Method
cpg	715.69	J/mol×K	887.78	Joback Method
cpg	727.82	J/mol×K	923.24	Joback Method
cpg	738.89	J/mol×K	958.69	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=U390717&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