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

Inchi: InChI=1S/C15H24O4/c1-6-8-12(7-2)19-14(17)10-9-13(16)18-11-15(3,4)5/h12H,7,9-11H2
InchiKey: PEMAPPXRABBIET-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: CC#CC(CC)OC(=O)CCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-189.22	kJ/mol	Joback Method
hf	-584.26	kJ/mol	Joback Method
hfus	32.36	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.701		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1712.00		NIST Webbook
tb	700.51	K	Joback Method
tc	901.64	K	Joback Method
tf	496.65	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.70	J/mol×K	700.51	Joback Method
cpg	651.93	J/mol×K	734.03	Joback Method
cpg	667.23	J/mol×K	767.55	Joback Method
cpg	681.60	J/mol×K	801.08	Joback Method
cpg	695.07	J/mol×K	834.60	Joback Method
cpg	707.67	J/mol×K	868.12	Joback Method
cpg	719.42	J/mol×K	901.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389580&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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