

Succinic acid, 2-methylpent-3-yl hex-5-en-1-yl ester

Inchi:	InChI=1S/C16H28O4/c1-5-7-8-9-12-19-15(17)10-11-16(18)20-14(6-2)13(3)4/h5,13-14H,1
InchiKey:	LBAZOEVHBRGJS-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	C=CCCCCOC(=O)CCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-301.04	kJ/mol	Joback Method
hf	-748.30	kJ/mol	Joback Method
hfus	34.44	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.644		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	713.86	K	Joback Method
tc	895.86	K	Joback Method
tf	382.64	K	Joback Method
vc	0.949	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.01	J/molxK	713.86	Joback Method
cpg	726.47	J/molxK	744.19	Joback Method
cpg	742.08	J/molxK	774.53	Joback Method
cpg	756.84	J/molxK	804.86	Joback Method
cpg	770.77	J/molxK	835.20	Joback Method
cpg	783.88	J/molxK	865.53	Joback Method
cpg	796.17	J/molxK	895.86	Joback Method
dvisc	0.0018739	Paxs	382.64	Joback Method

dvisc	0.0008051	Paxs	437.84	Joback Method
dvisc	0.0004179	Paxs	493.05	Joback Method
dvisc	0.0002476	Paxs	548.25	Joback Method
dvisc	0.0001614	Paxs	603.45	Joback Method
dvisc	0.0001130	Paxs	658.66	Joback Method
dvisc	0.0000837	Paxs	713.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391280&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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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