

Succinic acid, 2-methylpent-3-yl but-3-en-1-yl ester

Inchi:	InChI=1S/C14H24O4/c1-5-7-10-17-13(15)8-9-14(16)18-12(6-2)11(3)4/h5,11-12H,1,6-10H
InchiKey:	ZVWULLAPTPTTEP-UHFFFAOYSA-N
Formula:	C14H24O4
SMILES:	C=CCCOC(=O)CCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-317.88	kJ/mol	Joback Method
hf	-707.02	kJ/mol	Joback Method
hfus	29.26	kJ/mol	Joback Method
hvap	63.62	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.864		Crippen Method
mvol	218.700	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	668.10	K	Joback Method
tc	851.38	K	Joback Method
tf	360.10	K	Joback Method
vc	0.837	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.88	J/molxK	668.10	Joback Method
cpg	670.28	J/molxK	820.83	Joback Method
cpg	657.72	J/molxK	790.28	Joback Method
cpg	644.41	J/molxK	759.74	Joback Method
cpg	630.33	J/molxK	729.19	Joback Method
cpg	615.49	J/molxK	698.65	Joback Method
cpg	682.09	J/molxK	851.38	Joback Method
dvisc	0.0001083	Paxs	668.10	Joback Method

dvisc	0.0001456	Paxs	616.77	Joback Method
dvisc	0.0002066	Paxs	565.43	Joback Method
dvisc	0.0003142	Paxs	514.10	Joback Method
dvisc	0.0005247	Paxs	462.77	Joback Method
dvisc	0.0009955	Paxs	411.43	Joback Method
dvisc	0.0022675	Paxs	360.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391188&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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