Succinic acid, 3-methylbut-2-yl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C16H30O4/c1-10(2)13(7)19-14(17)8-9-15(18)20-16(11(3)4)12(5)6/h10-13,16H

InchiKey: JHTDETHEIMKBHJ-UHFFFAOYSA-N

Formula: C16H30O4

SMILES: CC(C)C(C)OC(=O)CCC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-396.20	kJ/mol	Joback Method
hf	-889.57	kJ/mol	Joback Method
hfus	25.16	kJ/mol	Joback Method
hvap	67.58	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.578		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
tb	715.86	K	Joback Method
tc	902.76	K	Joback Method
tf	339.40	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.99	J/mol×K	715.86	Joback Method
cpg	753.67	J/mol×K	747.01	Joback Method
cpg	770.38	J/mol×K	778.16	Joback Method
cpg	786.15	J/mol×K	809.31	Joback Method
cpg	800.97	J/mol×K	840.46	Joback Method
cpg	814.87	J/mol×K	871.61	Joback Method
cpg	827.84	J/mol×K	902.76	Joback Method
dvisc	0.0043758	Pa×s	339.40	Joback Method

dvisc	0.0012402	Pa×s	402.14	Joback Method
dvisc	0.0004940	Pa×s	464.89	Joback Method
dvisc	0.0002449	Pa×s	527.63	Joback Method
dvisc	0.0001410	Pa×s	590.37	Joback Method
dvisc	0.0000902	Pa×s	653.12	Joback Method
dvisc	0.0000624	Pa×s	715.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390502&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
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