Succinic acid, 3-methylbut-2-yl 2-methylpent-3-yl ester

Inchi: InChI=1S/C15H28O4/c1-7-13(11(4)5)19-15(17)9-8-14(16)18-12(6)10(2)3/h10-13H,7-9H2

InchiKey: PHWJAKCMZLYEQR-UHFFFAOYSA-N

Formula: C15H28O4

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

Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-402.18	kJ/mol	Joback Method
hf	-863.65	kJ/mol	Joback Method
hfus	26.09	kJ/mol	Joback Method
hvap	65.74	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.332		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	693.42	K	Joback Method
tc	878.58	K	Joback Method
tf	343.13	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.17	J/mol×K	693.42	Joback Method
cpg	755.78	J/mol×K	847.72	Joback Method
cpg	742.20	J/mol×K	816.86	Joback Method
cpg	727.76	J/mol×K	786.00	Joback Method
cpg	712.44	J/mol×K	755.14	Joback Method
cpg	696.25	J/mol×K	724.28	Joback Method
cpg	768.51	J/mol×K	878.58	Joback Method
dvisc	0.0000775	Pa×s	693.42	Joback Method

dvisc	0.0001096	Pa×s	635.04	Joback Method
dvisc	0.0001662	Pa×s	576.66	Joback Method
dvisc	0.0002767	Pa×s	518.27	Joback Method
dvisc	0.0005245	Pa×s	459.89	Joback Method
dvisc	0.0011973	Pa×s	401.51	Joback Method
dvisc	0.0036197	Pa×s	343.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/90-110-9/Succinic-acid-3-methylbut-2-yl-2-methylpent-3-yl-ester.pdf
Generated by Cheméo on 2024-10-12 02:38:00.641950892 +0000 UTC m=+3281543.278920141.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.