Succinic acid, 2-methylpent-3-yl 4-methylpent-2-yl ester

Inchi: InChI=1S/C16H30O4/c1-7-14(12(4)5)20-16(18)9-8-15(17)19-13(6)10-11(2)3/h11-14H,7-1

InchiKey: FJDJGJOYSOVIHT-UHFFFAOYSA-N

Formula: C16H30O4

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

Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-393.76	kJ/mol	Joback Method
hf	-884.29	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	67.97	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.722		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	1683.00		NIST Webbook
rinpol	1683.00		NIST Webbook
tb	716.30	K	Joback Method
tc	900.82	K	Joback Method
tf	354.40	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.52	J/mol×K	716.30	Joback Method
cpg	752.94	J/mol×K	747.05	Joback Method
cpg	769.44	J/mol×K	777.81	Joback Method
cpg	785.03	J/mol×K	808.56	Joback Method
cpg	799.71	J/mol×K	839.31	Joback Method
cpg	813.48	J/mol×K	870.06	Joback Method
cpg	826.37	J/mol×K	900.82	Joback Method
dvisc	0.0031943	Pa×s	354.40	Joback Method

dvisc	0.0010527	Pa×s	414.72	Joback Method
dvisc	0.0004599	Pa×s	475.03	Joback Method
dvisc	0.0002421	Pa×s	535.35	Joback Method
dvisc	0.0001452	Pa×s	595.67	Joback Method
dvisc	0.0000956	Pa×s	655.98	Joback Method
dvisc	0.0000676	Pa×s	716.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390425&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