Succinic acid, 2,2-dimethylpent-3-yl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H34O4/c1-8-10-14(13(3)4)21-16(19)11-12-17(20)22-15(9-2)18(5,6)7/h13-1

InchiKey: MEKHWZUEHDDYIU-UHFFFAOYSA-N

Formula: C18H34O4

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

Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-371.64	kJ/mol	Joback Method
hf	-929.04	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	71.51	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.502		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	759.27	K	Joback Method
tc	947.34	K	Joback Method
tf	394.36	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.50	J/mol×K	759.27	Joback Method
cpg	870.61	J/mol×K	790.61	Joback Method
cpg	887.68	J/mol×K	821.96	Joback Method
cpg	903.72	J/mol×K	853.30	Joback Method
cpg	918.78	J/mol×K	884.65	Joback Method
cpg	932.87	J/mol×K	915.99	Joback Method
cpg	946.02	J/mol×K	947.34	Joback Method
dvisc	0.0019641	Pa×s	394.36	Joback Method

dvisc	0.0006880	Pa×s	455.18	Joback Method
dvisc	0.0003086	Pa×s	516.00	Joback Method
dvisc	0.0001640	Pa×s	576.82	Joback Method
dvisc	0.0000983	Pa×s	637.63	Joback Method
dvisc	0.0000644	Pa×s	698.45	Joback Method
dvisc	0.0000451	Pa×s	759.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381733&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