

Succinic acid, 2-methylhex-3-yl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C19H36O4/c1-8-9-16(14(2)3)23-18(21)11-10-17(20)22-13-15(4)12-19(5,6)7/h1
InchiKey:	FBRSKTLZGVNKIT-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCCC(OC(=O)CCC(=O)OCC(C)CC(C)(C)C)C(C)C
Mol. weight [g/mol]:	328.49

Physical Properties

Property code	Value	Unit	Source
gf	-363.22	kJ/mol	Joback Method
hf	-949.68	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	73.74	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.750		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	782.15	K	Joback Method
tc	970.65	K	Joback Method
tf	405.63	K	Joback Method
vc	1.119	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.64	J/molxK	782.15	Joback Method
cpg	929.99	J/molxK	813.57	Joback Method
cpg	947.26	J/molxK	844.98	Joback Method
cpg	963.49	J/molxK	876.40	Joback Method
cpg	978.69	J/molxK	907.82	Joback Method
cpg	992.90	J/molxK	939.23	Joback Method
cpg	1006.14	J/molxK	970.65	Joback Method
dvisc	0.0017052	Paxs	405.63	Joback Method

dvisc	0.0005945	Paxs	468.38	Joback Method
dvisc	0.0002659	Paxs	531.14	Joback Method
dvisc	0.0001410	Paxs	593.89	Joback Method
dvisc	0.0000844	Paxs	656.64	Joback Method
dvisc	0.0000552	Paxs	719.40	Joback Method
dvisc	0.0000387	Paxs	782.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381321&Units=SI

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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