

Succinic acid, heptyl 3-oxobut-2-yl ester

Inchi:	InChI=1S/C15H26O5/c1-4-5-6-7-8-11-19-14(17)9-10-15(18)20-13(3)12(2)16/h13H,4-11H
InchiKey:	DPQWAFARYZTKTJ-UHFFFAOYSA-N
Formula:	C15H26O5
SMILES:	CCCCCCCOC(=O)CCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	286.36

Physical Properties

Property code	Value	Unit	Source
gf	-523.78	kJ/mol	Joback Method
hf	-960.39	kJ/mol	Joback Method
hfus	38.26	kJ/mol	Joback Method
hvap	73.65	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.801		Crippen Method
mcvol	238.660	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinsol	1918.00		NIST Webbook
tb	748.61	K	Joback Method
tc	934.38	K	Joback Method
tf	438.06	K	Joback Method
vc	0.923	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.93	J/molxK	748.61	Joback Method
cpg	715.00	J/molxK	779.57	Joback Method
cpg	729.20	J/molxK	810.53	Joback Method
cpg	742.56	J/molxK	841.50	Joback Method
cpg	755.07	J/molxK	872.46	Joback Method
cpg	766.74	J/molxK	903.42	Joback Method
cpg	777.57	J/molxK	934.38	Joback Method
dvisc	0.0012734	Paxs	438.06	Joback Method
dvisc	0.0006570	Paxs	489.82	Joback Method

dvisc	0.0003847	Paxs	541.58	Joback Method
dvisc	0.0002473	Paxs	593.34	Joback Method
dvisc	0.0001706	Paxs	645.09	Joback Method
dvisc	0.0001244	Paxs	696.85	Joback Method
dvisc	0.0000948	Paxs	748.61	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=U349582&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	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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