

Sebacic acid, 3-oxobut-2-yl propyl ester

Inchi:	InChI=1S/C17H30O5/c1-4-13-21-16(19)11-9-7-5-6-8-10-12-17(20)22-15(3)14(2)18/h15H
InchiKey:	HALMSEXUASPVKU-UHFFFAOYSA-N
Formula:	C17H30O5
SMILES:	CCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	314.42

Physical Properties

Property code	Value	Unit	Source
gf	-506.94	kJ/mol	Joback Method
hf	-1001.67	kJ/mol	Joback Method
hfus	43.44	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.581		Crippen Method
mcvol	266.840	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinqol	2166.00		NIST Webbook
tb	794.37	K	Joback Method
tc	981.67	K	Joback Method
tf	460.60	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.28	J/molxK	794.37	Joback Method
cpg	830.08	J/molxK	825.59	Joback Method
cpg	844.92	J/molxK	856.80	Joback Method
cpg	858.81	J/molxK	888.02	Joback Method
cpg	871.76	J/molxK	919.24	Joback Method
cpg	883.78	J/molxK	950.45	Joback Method
cpg	894.88	J/molxK	981.67	Joback Method
dvisc	0.0010403	Paxs	460.60	Joback Method
dvisc	0.0005239	Paxs	516.23	Joback Method

dvisc	0.0003015	Paxs	571.86	Joback Method
dvisc	0.0001914	Paxs	627.49	Joback Method
dvisc	0.0001308	Paxs	683.11	Joback Method
dvisc	0.0000947	Paxs	738.74	Joback Method
dvisc	0.0000717	Paxs	794.37	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=U355773&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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