

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

Inchi: InChI=1S/C19H34O5/c1-4-5-6-7-8-9-10-11-12-15-23-18(21)13-14-19(22)24-17(3)16(2)20
InchiKey: PPGRZQONRAZEEG-UHFFFAOYSA-N
Formula: C19H34O5
SMILES: CCCCCCCCCCOC(=O)CCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 342.47

Physical Properties

Property code	Value	Unit	Source
gf	-490.10	kJ/mol	Joback Method
hf	-1042.95	kJ/mol	Joback Method
hfus	48.62	kJ/mol	Joback Method
hvap	82.56	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.361		Crippen Method
mvol	295.020	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook
tb	840.13	K	Joback Method
tc	1031.64	K	Joback Method
tf	483.14	K	Joback Method
vc	1.147	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.24	J/molxK	840.13	Joback Method
cpg	948.74	J/molxK	872.05	Joback Method
cpg	964.15	J/molxK	903.97	Joback Method
cpg	978.50	J/molxK	935.88	Joback Method
cpg	991.79	J/molxK	967.80	Joback Method
cpg	1004.05	J/molxK	999.72	Joback Method
cpg	1015.28	J/molxK	1031.64	Joback Method
dvisc	0.0008351	Paxs	483.14	Joback Method

dvisc	0.0004114	Paxs	542.64	Joback Method
dvisc	0.0002331	Paxs	602.14	Joback Method
dvisc	0.0001463	Paxs	661.63	Joback Method
dvisc	0.0000991	Paxs	721.13	Joback Method
dvisc	0.0000713	Paxs	780.63	Joback Method
dvisc	0.0000537	Paxs	840.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349586&Units=SI
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

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
mccvol:	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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