

Succinic acid, hept-2-yl oct-1-en-3-yl ester

Inchi: InChI=1S/C19H34O4/c1-5-8-10-12-16(4)22-18(20)14-15-19(21)23-17(7-3)13-11-9-6-2/h
InchiKey: ZDGHYTIKWPYSZIW-UHFFFAOYSA-N
Formula: C19H34O4
SMILES: C=CC(CCCCC)OC(=O)CCC(=O)OC(C)CCCC
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-275.78	kJ/mol	Joback Method
hf	-810.22	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	74.75	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.957		Crippen Method
mvol	289.150	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	782.50	K	Joback Method
tc	966.47	K	Joback Method
tf	416.45	K	Joback Method
vc	1.117	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.50	J/molxK	782.50	Joback Method
cpg	901.04	J/molxK	813.16	Joback Method
cpg	917.59	J/molxK	843.82	Joback Method
cpg	933.16	J/molxK	874.48	Joback Method
cpg	947.78	J/molxK	905.15	Joback Method
cpg	961.47	J/molxK	935.81	Joback Method
cpg	974.23	J/molxK	966.47	Joback Method
dvisc	0.0013543	Paxs	416.45	Joback Method

dvisc	0.0005655	Paxs	477.46	Joback Method
dvisc	0.0002878	Paxs	538.47	Joback Method
dvisc	0.0001680	Paxs	599.48	Joback Method
dvisc	0.0001084	Paxs	660.48	Joback Method
dvisc	0.0000753	Paxs	721.49	Joback Method
dvisc	0.0000553	Paxs	782.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391320&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
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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