

Succinic acid, 2-ethylhexyl pent-4-en-2-yl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C17H30O4/c1-5-8-10-15(7-3)13-20-16(18)11-12-17(19)21-14(4)9-6-2/h6,14-15

CEIZJUIOPRJQAA-UHFFFAOYSA-N

C17H30O4

C=CCC(C)OC(=O)CCC(=O)OCC(CC)CCCC

298.42

Physical Properties

Property code	Value	Unit	Source
gf	-292.62	kJ/mol	Joback Method
hf	-768.94	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	70.30	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.034		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	736.74	K	Joback Method
tc	918.83	K	Joback Method
tf	393.91	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.82	J/mol×K	736.74	Joback Method
cpg	842.16	J/mol×K	888.48	Joback Method
cpg	828.83	J/mol×K	858.13	Joback Method
cpg	814.65	J/mol×K	827.78	Joback Method
cpg	799.59	J/mol×K	797.44	Joback Method
cpg	783.65	J/mol×K	767.09	Joback Method
cpg	854.64	J/mol×K	918.83	Joback Method
dvisc	0.0000731	Pa×s	736.74	Joback Method

dvisc	0.0000990	Pa×s	679.60	Joback Method
dvisc	0.0001418	Pa×s	622.46	Joback Method
dvisc	0.0002183	Pa×s	565.33	Joback Method
dvisc	0.0003705	Pa×s	508.19	Joback Method
dvisc	0.0007187	Pa×s	451.05	Joback Method
dvisc	0.0016896	Pa×s	393.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U391159&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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