

Succinic acid, 2-ethylhexyl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi: InChI=1S/C20H34O4/c1-4-6-10-17(5-2)14-23-19(21)12-13-20(22)24-15-18-11-8-7-9-16(

InchiKey: HCZTZWNTDLIZQI-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CCCCC(CC)COC(=O)CCC(=O)OCC1=C(C)CCCC1

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-309.90	kJ/mol	Joback Method
hf	-841.51	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.960		Crippen Method
mvol	292.380	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	2423.00		NIST Webbook
rinpol	2423.00		NIST Webbook
tb	842.48	K	Joback Method
tc	1042.81	K	Joback Method
tf	481.90	K	Joback Method
vc	1.117	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.80	J/molxK	842.48	Joback Method
cpg	1011.27	J/molxK	1009.42	Joback Method
cpg	998.39	J/molxK	976.03	Joback Method
cpg	984.32	J/molxK	942.64	Joback Method
cpg	969.04	J/molxK	909.26	Joback Method
cpg	952.54	J/molxK	875.87	Joback Method
cpg	1022.99	J/molxK	1042.81	Joback Method
dvisc	0.0000432	Paxs	842.48	Joback Method

dvisc	0.0000575	Paxs	782.38	Joback Method
dvisc	0.0000803	Paxs	722.29	Joback Method
dvisc	0.0001192	Paxs	662.19	Joback Method
dvisc	0.0001913	Paxs	602.09	Joback Method
dvisc	0.0003412	Paxs	542.00	Joback Method
dvisc	0.0007030	Paxs	481.90	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=U391419&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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