

Succinic acid, dodec-2-en-1-yl tetrahydrofurfuryl ester

Inchi: InChI=1S/C21H36O5/c1-2-3-4-5-6-7-8-9-10-11-16-25-20(22)14-15-21(23)26-18-19-13-12
InchiKey: BHQWTIIUUZDVEM-ZHACJKMWSA-N
Formula: C21H36O5
SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)OCC1CCCO1
Mol. weight [g/mol]: 368.51

Physical Properties

Property code	Value	Unit	Source
gf	-311.25	kJ/mol	Joback Method
hf	-920.67	kJ/mol	Joback Method
hfus	57.84	kJ/mol	Joback Method
hvap	85.38	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.729		Crippen Method
mcvol	312.340	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2850.00		NIST Webbook
rinpol	2850.00		NIST Webbook
tb	878.85	K	Joback Method
tc	1079.84	K	Joback Method
tf	503.14	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.64	J/mol×K	878.85	Joback Method
cpg	1049.33	J/mol×K	912.35	Joback Method
cpg	1065.82	J/mol×K	945.85	Joback Method
cpg	1081.13	J/mol×K	979.35	Joback Method
cpg	1095.32	J/mol×K	1012.85	Joback Method
cpg	1108.44	J/mol×K	1046.34	Joback Method
cpg	1120.51	J/mol×K	1079.84	Joback Method
dvisc	0.0007362	Pa×s	503.14	Joback Method

dvisc	0.0003691	Pa×s	565.76	Joback Method
dvisc	0.0002124	Pa×s	628.38	Joback Method
dvisc	0.0001351	Pa×s	691.00	Joback Method
dvisc	0.0000926	Pa×s	753.61	Joback Method
dvisc	0.0000673	Pa×s	816.23	Joback Method
dvisc	0.0000512	Pa×s	878.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U390728&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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