

Succinic acid, cyclohexylmethyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C16H26O5/c17-15(20-11-13-5-2-1-3-6-13)8-9-16(18)21-12-14-7-4-10-19-14/h1-16
InchiKey: HRRHGXLBOUYAL-UHFFFAOYSA-N
Formula: C16H26O5
SMILES: O=C(CCC(=O)OCC1CCCO1)OCC1CCCCC1
Mol. weight [g/mol]: 298.37

Physical Properties

Property code	Value	Unit	Source
gf	-409.12	kJ/mol	Joback Method
hf	-880.37	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.612		Crippen Method
mcvol	235.330	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook
tb	779.84	K	Joback Method
tc	995.61	K	Joback Method
tf	459.25	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.16	J/mol×K	779.84	Joback Method
cpg	773.87	J/mol×K	815.80	Joback Method
cpg	791.15	J/mol×K	851.76	Joback Method
cpg	807.01	J/mol×K	887.72	Joback Method
cpg	821.48	J/mol×K	923.68	Joback Method
cpg	834.59	J/mol×K	959.65	Joback Method
cpg	846.37	J/mol×K	995.61	Joback Method
dvisc	0.0015403	Pa×s	459.25	Joback Method

dvisc	0.0008130	Pa×s	512.68	Joback Method
dvisc	0.0004842	Pa×s	566.11	Joback Method
dvisc	0.0003153	Pa×s	619.55	Joback Method
dvisc	0.0002198	Pa×s	672.98	Joback Method
dvisc	0.0001616	Pa×s	726.41	Joback Method
dvisc	0.0001239	Pa×s	779.84	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=U390720&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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