

Succinic acid, cyclohexylmethyl 1-cyclopentylethyl ester

Inchi: InChI=1S/C18H30O4/c1-14(16-9-5-6-10-16)22-18(20)12-11-17(19)21-13-15-7-3-2-4-8-15
InchiKey: LHWJATSHKCPYLT-UHFFFAOYSA-N
Formula: C18H30O4
SMILES: CC(OC(=O)CCC(=O)OCC1CCCCC1)C1CCCC1
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-308.60	kJ/mol	Joback Method
hf	-794.93	kJ/mol	Joback Method
hfus	30.20	kJ/mol	Joback Method
hvap	74.27	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.012		Crippen Method
mvol	257.640	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	798.21	K	Joback Method
tc	1013.65	K	Joback Method
tf	440.22	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.92	J/molxK	798.21	Joback Method
cpg	858.93	J/molxK	834.12	Joback Method
cpg	877.40	J/molxK	870.02	Joback Method
cpg	894.36	J/molxK	905.93	Joback Method
cpg	909.85	J/molxK	941.84	Joback Method
cpg	923.91	J/molxK	977.74	Joback Method
cpg	936.56	J/molxK	1013.65	Joback Method
dvisc	0.0017454	Paxs	440.22	Joback Method

dvisc	0.0008136	Paxs	499.88	Joback Method
dvisc	0.0004463	Paxs	559.55	Joback Method
dvisc	0.0002749	Paxs	619.22	Joback Method
dvisc	0.0001843	Paxs	678.88	Joback Method
dvisc	0.0001319	Paxs	738.55	Joback Method
dvisc	0.0000992	Paxs	798.21	Joback Method

Sources

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=U391413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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