

Succinic acid, cyclohexylmethyl 4-acetylphenyl ester

Inchi: InChI=1S/C19H24O5/c1-14(20)16-7-9-17(10-8-16)24-19(22)12-11-18(21)23-13-15-5-3-2
InchiKey: AWODAOUOPYKZTQ-UHFFFAOYSA-N
Formula: C19H24O5
SMILES: CC(=O)c1ccc(OC(=O)CCC(=O)OCC2CCCCC2)cc1
Mol. weight [g/mol]: 332.39

Physical Properties

Property code	Value	Unit	Source
gf	-360.43	kJ/mol	Joback Method
hf	-758.29	kJ/mol	Joback Method
hfus	37.63	kJ/mol	Joback Method
hvap	86.31	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.698		Crippen Method
mcvol	260.400	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2789.00		NIST Webbook
tb	891.78	K	Joback Method
tc	1118.83	K	Joback Method
tf	544.46	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.25	J/mol×K	891.78	Joback Method
cpg	843.90	J/mol×K	929.62	Joback Method
cpg	857.03	J/mol×K	967.46	Joback Method
cpg	868.67	J/mol×K	1005.30	Joback Method
cpg	878.84	J/mol×K	1043.15	Joback Method
cpg	887.59	J/mol×K	1080.99	Joback Method
cpg	894.93	J/mol×K	1118.83	Joback Method
dvisc	0.0006112	Pa×s	544.46	Joback Method
dvisc	0.0003481	Pa×s	602.35	Joback Method

dvisc	0.0002189	Pa×s	660.23	Joback Method
dvisc	0.0001483	Pa×s	718.12	Joback Method
dvisc	0.0001065	Pa×s	776.01	Joback Method
dvisc	0.0000801	Pa×s	833.89	Joback Method
dvisc	0.0000625	Pa×s	891.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389913&Units=SI
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

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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