

Succinic acid, cyclohexylmethyl 4-octyl ester

Inchi:	InChI=1S/C19H34O4/c1-3-5-12-17(9-4-2)23-19(21)14-13-18(20)22-15-16-10-7-6-8-11-16
InchiKey:	KQBZLNGYJQJZFT-UHFFFAOYSA-N
Formula:	C19H34O4
SMILES:	CCCCC(CCC)OC(=O)CCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-336.73	kJ/mol	Joback Method
hf	-876.05	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	76.24	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.792		Crippen Method
mvol	282.590	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	805.81	K	Joback Method
tc	1002.74	K	Joback Method
tf	440.59	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.26	J/molxK	805.81	Joback Method
cpg	925.21	J/molxK	838.63	Joback Method
cpg	942.89	J/molxK	871.45	Joback Method
cpg	959.30	J/molxK	904.28	Joback Method
cpg	974.49	J/molxK	937.10	Joback Method
cpg	988.46	J/molxK	969.92	Joback Method
cpg	1001.23	J/molxK	1002.74	Joback Method
dvisc	0.0012775	Paxs	440.59	Joback Method

dvisc	0.0005593	Paxs	501.46	Joback Method
dvisc	0.0002928	Paxs	562.33	Joback Method
dvisc	0.0001739	Paxs	623.20	Joback Method
dvisc	0.0001134	Paxs	684.07	Joback Method
dvisc	0.0000792	Paxs	744.94	Joback Method
dvisc	0.0000585	Paxs	805.81	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=U389563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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