

Succinic acid, cyclohexylmethyl 3-methoxyphenyl ester

Inchi:	InChI=1S/C18H24O5/c1-21-15-8-5-9-16(12-15)23-18(20)11-10-17(19)22-13-14-6-3-2-4-7
InchiKey:	LIPFZQXQRYMVCV-UHFFFAOYSA-N
Formula:	C18H24O5
SMILES:	COc1cccc(OC(=O)CCC(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]:	320.38

Physical Properties

Property code	Value	Unit	Source
gf	-344.93	kJ/mol	Joback Method
hf	-757.29	kJ/mol	Joback Method
hfus	34.62	kJ/mol	Joback Method
hvap	79.75	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.504		Crippen Method
mvol	250.610	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
tb	837.45	K	Joback Method
tc	1059.18	K	Joback Method
tf	505.49	K	Joback Method
vc	0.934	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.54	J/molxK	837.45	Joback Method
cpg	800.83	J/molxK	874.40	Joback Method
cpg	815.61	J/molxK	911.36	Joback Method
cpg	828.91	J/molxK	948.31	Joback Method
cpg	840.72	J/molxK	985.27	Joback Method
cpg	851.05	J/molxK	1022.22	Joback Method
cpg	859.93	J/molxK	1059.18	Joback Method
dvisc	0.0005796	Paxs	505.49	Joback Method

dvisc	0.0003246	Paxs	560.82	Joback Method
dvisc	0.0002017	Paxs	616.14	Joback Method
dvisc	0.0001356	Paxs	671.47	Joback Method
dvisc	0.0000968	Paxs	726.80	Joback Method
dvisc	0.0000725	Paxs	782.12	Joback Method
dvisc	0.0000564	Paxs	837.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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