

Succinic acid, cyclohexylmethyl hept-1,6-dien-4-yl ester

Inchi: InChI=1S/C18H28O4/c1-3-8-16(9-4-2)22-18(20)13-12-17(19)21-14-15-10-6-5-7-11-15/h3-17,21-22H,18-20H2,19H3
InchiKey: HRUVINYFRULCNB-UHFFFAOYSA-N
Formula: C18H28O4
SMILES: C=CCC(CC=C)OC(=O)CCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-169.47	kJ/mol	Joback Method
hf	-604.55	kJ/mol	Joback Method
hfus	33.70	kJ/mol	Joback Method
hvap	72.67	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.954		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	776.29	K	Joback Method
tc	977.84	K	Joback Method
tf	425.80	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.10	J/molxK	776.29	Joback Method
cpg	872.00	J/molxK	944.25	Joback Method
cpg	858.73	J/molxK	910.66	Joback Method
cpg	844.33	J/molxK	877.06	Joback Method
cpg	828.78	J/molxK	843.47	Joback Method
cpg	812.05	J/molxK	809.88	Joback Method
cpg	884.16	J/molxK	977.84	Joback Method
dvisc	0.0000765	Paxs	776.29	Joback Method

dvisc	0.0001023	Paxs	717.88	Joback Method
dvisc	0.0001440	Paxs	659.46	Joback Method
dvisc	0.0002167	Paxs	601.04	Joback Method
dvisc	0.0003562	Paxs	542.63	Joback Method
dvisc	0.0006599	Paxs	484.21	Joback Method
dvisc	0.0014480	Paxs	425.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391333&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

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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