

Succinic acid, cyclohexylmethyl but-3-en-1-yl ester

Inchi: InChI=1S/C15H24O4/c1-2-3-11-18-14(16)9-10-15(17)19-12-13-7-5-4-6-8-13/h2,13H,1,3-
InchiKey: SCZIAVXEJINFCR-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: C=CCCOC(=O)CCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-280.13	kJ/mol	Joback Method
hf	-662.78	kJ/mol	Joback Method
hfus	30.73	kJ/mol	Joback Method
hvap	67.05	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.009		Crippen Method
mcvol	221.930	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1926.00		NIST Webbook
tb	711.41	K	Joback Method
tc	912.13	K	Joback Method
tf	408.75	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.46	J/mol×K	711.41	Joback Method
cpg	665.10	J/mol×K	744.86	Joback Method
cpg	681.65	J/mol×K	778.32	Joback Method
cpg	697.12	J/mol×K	811.77	Joback Method
cpg	711.53	J/mol×K	845.22	Joback Method
cpg	724.89	J/mol×K	878.68	Joback Method
cpg	737.22	J/mol×K	912.13	Joback Method
dvisc	0.0016041	Pa×s	408.75	Joback Method
dvisc	0.0008152	Pa×s	459.19	Joback Method

dvisc	0.0004737	Pa×s	509.64	Joback Method
dvisc	0.0003035	Pa×s	560.08	Joback Method
dvisc	0.0002093	Pa×s	610.52	Joback Method
dvisc	0.0001528	Pa×s	660.97	Joback Method
dvisc	0.0001166	Pa×s	711.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391195&Units=SI

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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