Succinic acid, cyclohexylmethyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C16H26O4/c1-13(2)10-11-19-15(17)8-9-16(18)20-12-14-6-4-3-5-7-14/h10,14H

InchiKey: NMZMZAPCRLGSJK-UHFFFAOYSA-N

Formula: C16H26O4

SMILES: CC(C)=CCOC(=O)CCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-287.88	kJ/mol	Joback Method
hf	-701.42	kJ/mol	Joback Method
hfus	33.50	kJ/mol	Joback Method
hvap	69.99	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.399		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	741.65	K	Joback Method
tc	946.50	K	Joback Method
tf	402.74	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.88	J/mol×K	741.65	Joback Method
cpg	722.96	J/mol×K	775.79	Joback Method
cpg	739.87	J/mol×K	809.93	Joback Method
cpg	755.65	J/mol×K	844.07	Joback Method
cpg	770.32	J/mol×K	878.22	Joback Method
cpg	783.92	J/mol×K	912.36	Joback Method
cpg	796.45	J/mol×K	946.50	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=U391036&Units=SI

Legend

cpg:	Ideal gas heat capacity
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