Succinic acid, cyclohexylmethyl 3-methylbut-3-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/h14H,1,3

InchiKey: KIKKVKOQTMTNTG-UHFFFAOYSA-N

Formula: C16H26O4

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

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-280.26	kJ/mol	Joback Method
hf	-693.21	kJ/mol	Joback Method
hfus	32.01	kJ/mol	Joback Method
hvap	69.36	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.399		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	734.17	K	Joback Method
tc	935.57	K	Joback Method
tf	406.06	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.53	J/mol×K	734.17	Joback Method
cpg	721.58	J/mol×K	767.74	Joback Method
cpg	738.49	J/mol×K	801.30	Joback Method
cpg	754.28	J/mol×K	834.87	Joback Method
cpg	768.95	J/mol×K	868.44	Joback Method
cpg	782.53	J/mol×K	902.00	Joback Method
cpg	795.04	J/mol×K	935.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391138&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
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