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

Inchi: InChI=1S/C16H28O4/c1-12(2)13(3)20-16(18)10-9-15(17)19-11-14-7-5-4-6-8-14/h12-14H

InchiKey: ZMDWVPSLRPMXPS-UHFFFAOYSA-N

Formula: C16H28O4

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

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-364.43	kJ/mol	Joback Method
hf	-819.41	kJ/mol	Joback Method
hfus	27.56	kJ/mol	Joback Method
hvap	69.17	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.478		Crippen Method
mcvol	240.320	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	736.73	K	Joback Method
tc	938.75	K	Joback Method
tf	391.78	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.92	J/mol×K	736.73	Joback Method
cpg	812.37	J/mol×K	905.08	Joback Method
cpg	798.26	J/mol×K	871.41	Joback Method
cpg	782.97	J/mol×K	837.74	Joback Method
cpg	766.49	J/mol×K	804.07	Joback Method
cpg	748.81	J/mol×K	770.40	Joback Method
cpg	825.33	J/mol×K	938.75	Joback Method
dvisc	0.0000823	Pa×s	736.73	Joback Method

dvisc	0.0001129	Pa×s	679.24	Joback Method
dvisc	0.0001643	Pa×s	621.75	Joback Method
dvisc	0.0002579	Pa×s	564.25	Joback Method
dvisc	0.0004487	Pa×s	506.76	Joback Method
dvisc	0.0008993	Pa×s	449.27	Joback Method
dvisc	0.0022105	Pa×s	391.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390585&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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