Succinic acid, cyclohexylmethyl neopentyl ester

Inchi: InChI=1S/C16H28O4/c1-16(2,3)12-20-15(18)10-9-14(17)19-11-13-7-5-4-6-8-13/h13H,4-1

InchiKey: RZYMETSMKGCZQR-UHFFFAOYSA-N

Formula: C16H28O4

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

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-356.71	kJ/mol	Joback Method
hf	-817.60	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	68.66	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.479		Crippen Method
mcvol	240.320	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	734.38	K	Joback Method
tc	938.90	K	Joback Method
tf	424.20	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.84	J/mol×K	734.38	Joback Method
cpg	812.90	J/mol×K	904.81	Joback Method
cpg	798.84	J/mol×K	870.72	Joback Method
cpg	783.63	J/mol×K	836.64	Joback Method
cpg	767.25	J/mol×K	802.55	Joback Method
cpg	749.67	J/mol×K	768.47	Joback Method
cpg	825.84	J/mol×K	938.90	Joback Method
dvisc	0.0000799	Pa×s	734.38	Joback Method

dvisc	0.0001080	Pa×s	682.68	Joback Method
dvisc	0.0001532	Pa×s	630.99	Joback Method
dvisc	0.0002315	Pa×s	579.29	Joback Method
dvisc	0.0003793	Pa×s	527.59	Joback Method
dvisc	0.0006918	Pa×s	475.90	Joback Method
dvisc	0.0014606	Pa×s	424.20	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=U389584&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