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

Inchi: InChI=1S/C17H30O4/c1-4-15(13(2)3)21-17(19)11-10-16(18)20-12-14-8-6-5-7-9-14/h13-1

InchiKey: AQEKVVAJKYGSPB-UHFFFAOYSA-N

Formula: C17H30O4

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

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-356.01	kJ/mol	Joback Method
hf	-840.05	kJ/mol	Joback Method
hfus	30.15	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.868		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	759.61	K	Joback Method
tc	960.07	K	Joback Method
tf	403.05	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.97	J/mol×K	759.61	Joback Method
cpg	870.69	J/mol×K	926.66	Joback Method
cpg	856.57	J/mol×K	893.25	Joback Method
cpg	841.26	J/mol×K	859.84	Joback Method
cpg	824.73	J/mol×K	826.43	Joback Method
cpg	806.97	J/mol×K	793.02	Joback Method
cpg	883.63	J/mol×K	960.07	Joback Method
dvisc	0.0000716	Pa×s	759.61	Joback Method

dvisc	0.0000984	Pa×s	700.18	Joback Method
dvisc	0.0001435	Pa×s	640.76	Joback Method
dvisc	0.0002260	Pa×s	581.33	Joback Method
dvisc	0.0003948	Pa×s	521.90	Joback Method
dvisc	0.0007958	Pa×s	462.48	Joback Method
dvisc	0.0019728	Pa×s	403.05	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=U389600&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