Succinic acid, naphth-2-ylmethyl cyclopentyl ester

Inchi: InChI=1S/C20H22O4/c21-19(11-12-20(22)24-18-7-3-4-8-18)23-14-15-9-10-16-5-1-2-6-17

InchiKey: MDTNOICUWQEEOM-UHFFFAOYSA-N

Formula: C20H22O4

SMILES: O=C(CCC(=O)OC1CCCC1)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-104.34	kJ/mol	Joback Method
hf	-469.12	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	83.26	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.149		Crippen Method
mcvol	253.460	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	875.50	K	Joback Method
tc	1108.22	K	Joback Method
tf	542.02	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.87	J/mol×K	875.50	Joback Method
cpg	808.05	J/mol×K	914.29	Joback Method
cpg	821.94	J/mol×K	953.07	Joback Method
cpg	834.62	J/mol×K	991.86	Joback Method
cpg	846.16	J/mol×K	1030.64	Joback Method
cpg	856.64	J/mol×K	1069.43	Joback Method
cpg	866.15	J/mol×K	1108.22	Joback Method
dvisc	0.0009662	Pa×s	542.02	Joback Method

dvisc	0.0006264	Pa×s	597.60	Joback Method
dvisc	0.0004372	Pa×s	653.18	Joback Method
dvisc	0.0003228	Pa×s	708.76	Joback Method
dvisc	0.0002491	Pa×s	764.34	Joback Method
dvisc	0.0001991	Pa×s	819.92	Joback Method
dvisc	0.0001638	Pa×s	875.50	Joback Method

Sources

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=U391387&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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