

Succinic acid, naphth-2-ylmethyl cis-4-methylcyclohexyl ester

Inchi:	InChI=1S/C22H26O4/c1-16-6-10-20(11-7-16)26-22(24)13-12-21(23)25-15-17-8-9-18-4-2
InchiKey:	JGSCGESOTFPLKS-UHFFFAOYSA-N
Formula:	C22H26O4
SMILES:	CC1CCC(OC(=O)CCC(=O)OCc2ccc3ccccc3c2)CC1
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-107.31	kJ/mol	Joback Method
hf	-536.90	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	87.58	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.785		Crippen Method
mvol	281.640	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
tb	920.86	K	Joback Method
tc	1154.06	K	Joback Method
tf	556.80	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.51	J/molxK	920.86	Joback Method
cpg	982.13	J/molxK	1115.20	Joback Method
cpg	972.19	J/molxK	1076.33	Joback Method
cpg	960.93	J/molxK	1037.46	Joback Method
cpg	948.27	J/molxK	998.59	Joback Method
cpg	934.15	J/molxK	959.73	Joback Method
cpg	990.81	J/molxK	1154.06	Joback Method
dvisc	0.0001142	Paxs	920.86	Joback Method

dvisc	0.0001402	Paxs	860.18	Joback Method
dvisc	0.0001776	Paxs	799.51	Joback Method
dvisc	0.0002339	Paxs	738.83	Joback Method
dvisc	0.0003236	Paxs	678.15	Joback Method
dvisc	0.0004771	Paxs	617.48	Joback Method
dvisc	0.0007657	Paxs	556.80	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=U390064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

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