

Succinic acid, naphth-2-ylmethyl trans-4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C25H32O4/c1-25(2,3)21-10-12-22(13-11-21)29-24(27)15-14-23(26)28-17-18-8
InchiKey:	PICAVKJZUHDXXKX-UHFFFAOYSA-N
Formula:	C25H32O4
SMILES:	CC(C)(C)C1CCC(OC(=O)CCC(=O)OCc2ccc3ccccc3c2)CC1
Mol. weight [g/mol]:	396.52

Physical Properties

Property code	Value	Unit	Source
gf	-79.21	kJ/mol	Joback Method
hf	-607.57	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	92.96	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	5.811		Crippen Method
mvol	323.910	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	3298.00		NIST Webbook
rinpol	3298.00		NIST Webbook
tb	986.27	K	Joback Method
tc	1223.20	K	Joback Method
tf	593.03	K	Joback Method
vc	1.218	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.32	J/molxK	986.27	Joback Method
cpg	1115.14	J/molxK	1025.76	Joback Method
cpg	1129.49	J/molxK	1065.25	Joback Method
cpg	1142.48	J/molxK	1104.74	Joback Method
cpg	1154.22	J/molxK	1144.23	Joback Method
cpg	1164.81	J/molxK	1183.72	Joback Method
cpg	1174.36	J/molxK	1223.20	Joback Method
dvisc	0.0004976	Paxs	593.03	Joback Method

dvisc	0.0002907	Paxs	658.57	Joback Method
dvisc	0.0001872	Paxs	724.11	Joback Method
dvisc	0.0001297	Paxs	789.65	Joback Method
dvisc	0.0000950	Paxs	855.19	Joback Method
dvisc	0.0000728	Paxs	920.73	Joback Method
dvisc	0.0000578	Paxs	986.27	Joback Method

Sources

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=U390205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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