

Succinic acid, naphth-2-ylmethyl 3,3-dimethylbut-2-yl ester

Inchi:	InChI=1S/C21H26O4/c1-15(21(2,3)4)25-20(23)12-11-19(22)24-14-16-9-10-17-7-5-6-8-18
InchiKey:	VOJCQFSLNSEFU-UHFFFAOYSA-N
Formula:	C21H26O4
SMILES:	CC(OC(=O)CCC(=O)OCc1ccc2ccccc2c1)C(C)(C)C
Mol. weight [g/mol]:	342.43

Physical Properties

Property code	Value	Unit	Source
gf	-132.07	kJ/mol	Joback Method
hf	-564.27	kJ/mol	Joback Method
hfus	35.45	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.641		Crippen Method
mcvol	278.410	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2698.00		NIST Webbook
tb	879.43	K	Joback Method
tc	1101.76	K	Joback Method
tf	529.81	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.41	J/molxK	879.43	Joback Method
cpg	927.31	J/molxK	1064.71	Joback Method
cpg	916.25	J/molxK	1027.65	Joback Method
cpg	904.32	J/molxK	990.60	Joback Method
cpg	891.42	J/molxK	953.54	Joback Method
cpg	877.47	J/molxK	916.49	Joback Method
cpg	937.57	J/molxK	1101.76	Joback Method
dvisc	0.0000679	Paxs	879.43	Joback Method
dvisc	0.0000864	Paxs	821.16	Joback Method

dvisc	0.0001140	Paxs	762.89	Joback Method
dvisc	0.0001576	Paxs	704.62	Joback Method
dvisc	0.0002310	Paxs	646.35	Joback Method
dvisc	0.0003652	Paxs	588.08	Joback Method
dvisc	0.0006385	Paxs	529.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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