

4a(2H)-naphthalenecarboxylic acid, octahydro-, trans-

Inchi: InChI=1S/C11H18O2/c12-10(13)11-7-3-1-5-9(11)6-2-4-8-11/h9H,1-8H2,(H,12,13)/t9-,11-
InchiKey: VAMBVWHKUJPMEB-JGZJWPJOSA-N
Formula: C11H18O2
SMILES: O=C(O)C12CCCCC1CCCC2
Mol. weight [g/mol]: 182.26
CAS: 2543-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-156.39	kJ/mol	Joback Method
hf	-398.98	kJ/mol	Joback Method
hfus	11.50	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.822		Crippen Method
mcvol	151.570	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	627.93	K	Joback Method
tc	846.57	K	Joback Method
tf	408.20 ± 2.00	K	NIST Webbook
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.13	J/mol×K	627.93	Joback Method
cpg	443.83	J/mol×K	664.37	Joback Method
cpg	459.50	J/mol×K	700.81	Joback Method
cpg	474.31	J/mol×K	737.25	Joback Method
cpg	488.40	J/mol×K	773.69	Joback Method
cpg	501.90	J/mol×K	810.13	Joback Method
cpg	514.96	J/mol×K	846.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2543751&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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