6,8-Dioxabicyclo[3.2.1]octane, 1,5-dimethyl-, (1S)-

Other names: (-)-Frontalin
(S)-(-)-Frontalin
(1S)-1,5-Dimethyl-6,8-dioxabicyclo[3.2.1]octane
Frontalin
6,8-Dioxabicyclo(3.2.1)octane, 1,5-dimethyl-
1,5-Dimethyl-6,8-dioxabicyclo(3.2.1)octane
(-)-(1S,5R)-Frontalin
Frontaline

Inchi: InChI=1S/C8H14O2/c1-7-4-3-5-8(2,10-7)9-6-7/h3-6H2,1-2H3

InchiKey: AZWKCIZRVUVZPX-UHFFFAOYSA-N

Formula: C8H14O2

SMILES: CC12CCCC(C)(OC1)O2

Mol. weight [g/mol]: 142.20

CAS: 28401-39-0

Physical Properties

Property code	Value	Unit	Source
gf	-69.44	kJ/mol	Joback Method
hf	-308.69	kJ/mol	Joback Method
hfus	11.91	kJ/mol	Joback Method
hvap	40.29	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.692		Crippen Method
mcvol	113.600	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	949.20		NIST Webbook
tb	458.84	K	Joback Method
tc	687.32	K	Joback Method
tf	309.70	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	264.03	J/mol×K	458.84	Joback Method
cpg	281.42	J/mol×K	496.92	Joback Method
cpg	297.06	J/mol×K	535.00	Joback Method
cpg	311.23	J/mol×K	573.08	Joback Method
cpg	324.18	J/mol×K	611.16	Joback Method
cpg	336.18	J/mol×K	649.24	Joback Method
cpg	347.50	J/mol×K	687.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28401390&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume