6,8-Dioxabicyclo[3.2.1]octane, 7-ethyl-5-methyl-, (1R-exo)-

Other names: exo-Brevicomin
Brevicomin
exo-7-Ethyl-5-methyl-6,8-dioxabicyclo[3.2.1]octane

Inchi: InChI=1S/C9H16O2/c1-3-7-8-5-4-6-9(2,10-7)11-8/h7-8H,3-6H2,1-2H3

InchiKey: YONXEBYXWVCXIV-UHFFFAOYSA-N

Formula: C9H16O2

SMILES: CCC1OC2(C)CCCC1O2

Mol. weight [g/mol]: 156.22

CAS: 20290-99-7

Physical Properties

Property code	Value	Unit	Source
gf	-63.24	kJ/mol	Joback Method
hf	-364.91	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	43.36	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.081		Crippen Method
mcvol	127.690	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	476.81	K	Joback Method
tc	691.82	K	Joback Method
tf	292.83	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.21	J/mol×K	476.81	Joback Method
cpg	326.46	J/mol×K	512.64	Joback Method
cpg	343.39	J/mol×K	548.48	Joback Method
cpg	359.13	J/mol×K	584.31	Joback Method
cpg	373.82	J/mol×K	620.15	Joback Method
cpg	387.60	J/mol×K	655.98	Joback Method

cpg	400.59	J/mol×K	691.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.50 ± 2.50	K	14.70	NIST Webbook

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=C20290997&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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