Anti-tricyclo[3.2.0.0(2,4)]heptane

Inchi: InChI=1S/C8H12/c1-8-4-7(8)5-2-3-6(5)8/h5-7H,2-4H2,1H3/t5-,6+,7+,8-/m0/s1
InchiKey: QDRDEZNWCZDAEJ-OSMVPFSASA-N
Formula: C7H10
SMILES: CC12CC1C1CCC12
Mol. weight [g/mol]: 94.15
CAS: 28102-61-6

Physical Properties

Property code	Value	Unit	Source
gf	209.73	kJ/mol	Joback Method
hf	235.00	kJ/mol	NIST Webbook
hfus	9.85	kJ/mol	Joback Method
hvap	31.34	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	2.052		Crippen Method
mcvol	91.000	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	389.69	K	Joback Method
tc	591.59	K	Joback Method
tf	260.44	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.81	J/mol×K	389.69	Joback Method
cpg	206.27	J/mol×K	423.34	Joback Method
cpg	222.07	J/mol×K	456.99	Joback Method
cpg	236.35	J/mol×K	490.64	Joback Method
cpg	249.29	J/mol×K	524.29	Joback Method
cpg	261.04	J/mol×K	557.94	Joback Method
cpg	271.77	J/mol×K	591.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28102616&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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