Tricyclo[8.3.0.0(4,9)]dodecane, isomer # 4

Inchi: InChI=1S/C13H22/c1-2-6-12-10(4-1)8-9-11-5-3-7-13(11)12/h10-13H,1-9H2
InchiKey: DDBLMNQGXGUZOS-UHFFFAOYSA-N
Formula: C13H22
SMILES: C1CCC2C(C1)CCC1CCCC12
Mol. weight [g/mol]: 178.31

Physical Properties

Property code	Value	Unit	Source
gf	184.72	kJ/mol	Joback Method
hf	-138.23	kJ/mol	Joback Method
hfus	16.50	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	4.003		Crippen Method
mcvol	161.450	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1444.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1647.00		NIST Webbook
tb	529.47	K	Joback Method
tc	757.82	K	Joback Method
tf	271.77	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.40	J/mol×K	529.47	Joback Method
cpg	534.62	J/mol×K	719.76	Joback Method
cpg	515.09	J/mol×K	681.70	Joback Method
cpg	494.09	J/mol×K	643.64	Joback Method
cpg	471.54	J/mol×K	605.59	Joback Method

cpg	447.35	J/mol×K	567.53	Joback Method
cpg	552.80	J/mol×K	757.82	Joback Method
dvisc	0.0008444	Pa×s	529.47	Joback Method
dvisc	0.0009322	Pa×s	486.52	Joback Method
dvisc	0.0010489	Pa×s	443.57	Joback Method
dvisc	0.0012105	Pa×s	400.62	Joback Method
dvisc	0.0014458	Pa×s	357.67	Joback Method
dvisc	0.0018128	Pa×s	314.72	Joback Method
dvisc	0.0024413	Pa×s	271.77	Joback Method

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=R524646&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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