(1S,2R,4R,7R)-4-Isopropyl-7-methyl-3,8-dioxatricy

Inchi: InChI=1S/C10H16O2/c1-6(2)10-5-4-9(3)7(11-9)8(10)12-10/h6-8H,4-5H2,1-3H3
InchiKey: LEZWCCRTFNBOBU-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC(C)C12CCC3(C)OC3C1O2
Mol. weight [g/mol]: 168.23
CAS: 1619-26-7

Physical Properties

Property code	Value	Unit	Source
gf	34.30	kJ/mol	Joback Method
hf	-284.31	kJ/mol	Joback Method
hfus	19.07	kJ/mol	Joback Method
hvap	43.44	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.731		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinpol	1302.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1309.90		NIST Webbook
rinpol	1306.00		NIST Webbook
tb	493.42	K	Joback Method
tc	711.67	K	Joback Method
tf	341.50	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.55	J/mol×K	493.42	Joback Method
cpg	358.15	J/mol×K	529.80	Joback Method
cpg	374.04	J/mol×K	566.17	Joback Method

cpg	388.50	J/mol×K	602.55	Joback Method
cpg	401.82	J/mol×K	638.92	Joback Method
cpg	414.29	J/mol×K	675.30	Joback Method
cpg	426.18	J/mol×K	711.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1619267&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/71-104-7/1S-2R-4R-7R-4-Isopropyl-7-methyl-3-8-dioxatricyclo-5-1-0-02-4-octane.pdf
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