6,6,10-Trimethyldecal-2-one

Inchi: InChI=1S/C13H22O/c1-12(2)7-4-8-13(3)9-10(14)5-6-11(12)13/h11H,4-9H2,1-3H3
InchiKey: YZILXDJWJHJLAM-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CC1(C)CCCC2(C)CC(=O)CCC12
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	-9.60	kJ/mol	Joback Method
hf	-318.25	kJ/mol	Joback Method
hfus	5.28	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.572		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1505.00		NIST Webbook
rinpol	1505.00		NIST Webbook
ripol	2068.00		NIST Webbook
ripol	2068.00		NIST Webbook
tb	591.03	K	Joback Method
tc	835.84	K	Joback Method
tf	369.85	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.88	J/mol×K	591.03	Joback Method
cpg	498.03	J/mol×K	631.83	Joback Method
cpg	519.78	J/mol×K	672.63	Joback Method
cpg	540.41	J/mol×K	713.43	Joback Method
cpg	560.19	J/mol×K	754.23	Joback Method
cpg	579.40	J/mol×K	795.03	Joback Method

cpg	598.32	J/mol×K	835.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228863&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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