2-pinen-10-yl isobutyrate

Other names:	Myrtenyl isobutyrate
Inchi:	InChI=1S/C14H22O2/c1-9(2)13(15)16-8-10-5-6-11-7-12(10)14(11,3)4/h5,9,11-12H,6-8H2
InchiKey:	HPAQTXNDJUZELN-UHFFFAOYSA-N
Formula:	C14H22O2
SMILES:	CC(C)C(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]:	222.32
CAS:	29021-37-2

Physical Properties

Property code	Value	Unit	Source
gf	-52.83	kJ/mol	Joback Method
hf	-401.72	kJ/mol	Joback Method
hfus	21.06	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.178		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1466.40		NIST Webbook
rinpol	1466.40		NIST Webbook
tb	613.03	K	Joback Method
tc	821.06	K	Joback Method
tf	370.00	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.27	J/mol×K	613.03	Joback Method
cpg	538.61	J/mol×K	647.70	Joback Method
cpg	555.96	J/mol×K	682.37	Joback Method
cpg	572.43	J/mol×K	717.04	Joback Method
cpg	588.17	J/mol×K	751.72	Joback Method
cpg	603.29	J/mol×K	786.39	Joback Method

cpg	617.93	J/mol×K	821.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29021372&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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