2-Isopropyl-5-methylhex-5-enoic acid

Inchi: InChI=1S/C10H18O2/c1-7(2)5-6-9(8(3)4)10(11)12/h8-9H,1,5-6H2,2-4H3,(H,11,12)
InchiKey: NVOBEWKGWWJTOA-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: C=C(C)CCC(C(=O)O)C(C)C
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-158.01	kJ/mol	Joback Method
hf	-409.46	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	59.91	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.700		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
ripol	2132.00		NIST Webbook
tb	569.93	K	Joback Method
tc	748.12	K	Joback Method
tf	267.49	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.15	J/mol×K	569.93	Joback Method
cpg	395.70	J/mol×K	599.63	Joback Method
cpg	407.66	J/mol×K	629.33	Joback Method
cpg	419.05	J/mol×K	659.03	Joback Method
cpg	429.88	J/mol×K	688.72	Joback Method
cpg	440.19	J/mol×K	718.42	Joback Method
cpg	449.98	J/mol×K	748.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326120&Units=SI

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