2-Ethylbutyryl chloride

Other names: Butanoyl chloride, 2-ethyl-
Butyryl chloride, 2-ethyl-
2-Ethylbutyroyl chloride
2-Ethylbutiryl chloride
Diethylacetyl chloride
Inchi: InChI=1S/C6H11ClO/c1-3-5(4-2)6(7)8/h5H,3-4H2,1-2H3
InchiKey: SMUKODJVMQOSAB-UHFFFAOYSA-N
Formula: C6H11ClO
SMILES: CCC(CC)C(=O)Cl
Mol. weight [g/mol]: 134.60
CAS: 2736-40-5

Physical Properties

Property code	Value	Unit	Source
gf	-143.65	kJ/mol	Joback Method
hf	-300.77	kJ/mol	Joback Method
hfus	13.57	kJ/mol	Joback Method
hvap	39.69	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	2.188		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	850.60		NIST Webbook
rinpol	850.60		NIST Webbook
tb	413.00 ± 6.00	K	NIST Webbook
tb	413.00 ± 6.00	K	NIST Webbook
tc	616.78	K	Joback Method
tf	222.23	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.52	J/mol×K	616.78	Joback Method

cpg	203.25	J/mol×K	427.54	Joback Method
cpg	213.38	J/mol×K	459.08	Joback Method
cpg	223.06	J/mol×K	490.62	Joback Method
cpg	232.30	J/mol×K	522.16	Joback Method
cpg	241.12	J/mol×K	553.70	Joback Method
cpg	249.52	J/mol×K	585.24	Joback Method
dvisc	0.0003354	Pa×s	427.54	Joback Method
dvisc	0.0059488	Pa×s	222.23	Joback Method
dvisc	0.0026756	Pa×s	256.45	Joback Method
dvisc	0.0014525	Pa×s	290.67	Joback Method
dvisc	0.0008968	Pa×s	324.88	Joback Method
dvisc	0.0006070	Pa×s	359.10	Joback Method
dvisc	0.0004397	Pa×s	393.32	Joback Method
hvapt	39.40	kJ/mol	362.50	NIST Webbook

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=C2736405&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
hvapt: Enthalpy of vaporization at a given temperature
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