2-Ethylbutyric acid, 2-nitrophenyl ester

Inchi: InChI=1S/C12H15NO4/c1-3-9(4-2)12(14)17-11-8-6-5-7-10(11)13(15)16/h5-9H,3-4H2,1-2
InchiKey: UCLLPEPMLBPFEX-UHFFFAOYSA-N
Formula: C12H15NO4
SMILES: CCC(CC)C(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 237.25

Physical Properties

Property code	Value	Unit	Source
gf	-47.87	kJ/mol	Joback Method
hf	-326.79	kJ/mol	Joback Method
hfus	31.11	kJ/mol	Joback Method
hvap	70.60	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.936		Crippen Method
mcvol	181.040	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	733.31	K	Joback Method
tc	966.01	K	Joback Method
tf	464.71	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.12	J/mol×K	733.31	Joback Method
cpg	511.61	J/mol×K	772.09	Joback Method
cpg	524.08	J/mol×K	810.88	Joback Method
cpg	535.55	J/mol×K	849.66	Joback Method
cpg	546.05	J/mol×K	888.45	Joback Method
cpg	555.62	J/mol×K	927.23	Joback Method
cpg	564.27	J/mol×K	966.01	Joback Method

Sources

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=U369865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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