Benzoic acid, 4-ethyl-, 4-cyanophenyl ester

Other names: 4-Ethylbenzoic acid, 4-cyanophenyl ester
Inchi: InChI=1S/C16H13NO2/c1-2-12-3-7-14(8-4-12)16(18)19-15-9-5-13(11-17)6-10-15/h3-10H
InchiKey: ULFIAHFQEURGOU-UHFFFAOYSA-N
Formula: C16H13NO2
SMILES: CCc1ccc(C(=O)Oc2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 251.28
CAS: 56131-48-7

Physical Properties

Property code	Value	Unit	Source
gf	188.66	kJ/mol	Joback Method
hf	-3.37	kJ/mol	Joback Method
hfus	28.79	kJ/mol	Joback Method
hvap	76.72	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.340		Crippen Method
mcvol	197.600	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	2167.00		NIST Webbook
rinpol	2167.00		NIST Webbook
tb	807.17	K	Joback Method
tc	1051.84	K	Joback Method
tf	485.11	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.11	J/mol×K	807.17	Joback Method
cpg	549.37	J/mol×K	847.95	Joback Method
cpg	560.52	J/mol×K	888.73	Joback Method
cpg	570.60	J/mol×K	929.50	Joback Method
cpg	579.66	J/mol×K	970.28	Joback Method
cpg	587.75	J/mol×K	1011.06	Joback Method

cpg	594.91	J/mol×K	1051.84	Joback Method

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=C56131487&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
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