

«gamma»-Ethyl-benzylacetaldehyde

Inchi:	InChI=1S/C11H14O/c1-2-10(9-12)8-11-6-4-3-5-7-11/h3-7,9-10H,2,8H2,1H3
InchiKey:	ROPNSYBZOVTZBB-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CCC(C=O)Cc1ccccc1
Mol. weight [g/mol]:	162.23

Physical Properties

Property code	Value	Unit	Source
gf	52.19	kJ/mol	Joback Method
hf	-124.70	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	48.69	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.454		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
ripol	1949.00		NIST Webbook
tb	525.98	K	Joback Method
tc	736.91	K	Joback Method
tf	267.15	K	Joback Method
vc	0.554	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.76	J/mol×K	525.98	Joback Method
cpg	337.60	J/mol×K	561.13	Joback Method
cpg	351.55	J/mol×K	596.29	Joback Method
cpg	364.65	J/mol×K	631.44	Joback Method
cpg	376.92	J/mol×K	666.60	Joback Method
cpg	388.41	J/mol×K	701.75	Joback Method
cpg	399.16	J/mol×K	736.91	Joback Method
dvisc	0.0048580	Paxs	267.15	Joback Method
dvisc	0.0021017	Paxs	310.29	Joback Method

dvisc	0.0011156	Paxs	353.43	Joback Method
dvisc	0.0006797	Paxs	396.56	Joback Method
dvisc	0.0004563	Paxs	439.70	Joback Method
dvisc	0.0003290	Paxs	482.84	Joback Method
dvisc	0.0002503	Paxs	525.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R303216&Units=SI

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
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

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