2,3-diphenylbut-2-enal

Inchi: InChI=1S/C16H14O/c1-13(14-8-4-2-5-9-14)16(12-17)15-10-6-3-7-11-15/h2-12H,1H3/b16
InchiKey: WXHYNUFLMJBDNT-DTQAZKPQSA-N
Formula: C16H14O
SMILES: CC(=C(C=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	272.26	kJ/mol	Joback Method
hf	111.55	kJ/mol	Joback Method
hfus	25.15	kJ/mol	Joback Method
hvap	62.60	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.816		Crippen Method
mcvol	186.050	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	671.42	K	Joback Method
tc	921.15	K	Joback Method
tf	331.92	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.72	J/mol×K	671.42	Joback Method
cpg	485.97	J/mol×K	713.04	Joback Method
cpg	500.86	J/mol×K	754.66	Joback Method
cpg	514.51	J/mol×K	796.28	Joback Method
cpg	527.03	J/mol×K	837.91	Joback Method
cpg	538.56	J/mol×K	879.53	Joback Method
cpg	549.20	J/mol×K	921.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R396837&Units=SI
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

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