«alpha»-Methylcinnamyl acetate

Inchi: InChI=1S/C12H14O2/c1-10(9-14-11(2)13)8-12-6-4-3-5-7-12/h3-8H,9H2,1-2H3/b10-8+
InchiKey: BWYPZPVVNMYMKA-CSKARUKUSA-N
Formula: C12H14O2
SMILES: CC(=O)OCC(C)=Cc1ccccc1
Mol. weight [g/mol]: 190.24
CAS: 72797-29-6

Physical Properties

Property code	Value	Unit	Source
gf	0.32	kJ/mol	Joback Method
hf	-191.85	kJ/mol	Joback Method
hfus	22.56	kJ/mol	Joback Method
hvap	53.78	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.653		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1484.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2158.00		NIST Webbook
tb	580.97	K	Joback Method
tc	799.81	K	Joback Method
tf	304.54	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.15	J/mol×K	580.97	Joback Method
cpg	389.04	J/mol×K	617.44	Joback Method
cpg	402.99	J/mol×K	653.92	Joback Method
cpg	416.04	J/mol×K	690.39	Joback Method
cpg	428.24	J/mol×K	726.86	Joback Method
cpg	439.62	J/mol×K	763.34	Joback Method

cpg	450.23	J/mol×K	799.81	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=C72797296&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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