«alpha»-Heptylcinnamic aldehyde

Inchi: InChI=1S/C16H22O/c1-2-3-4-5-7-12-16(14-17)13-15-10-8-6-9-11-15/h6,8-11,13-14H,2-5
InchiKey: VXDUTTLHVAAEFQ-DTQAZKPQSA-N
Formula: C16H22O
SMILES: CCCCCCCC(C=O)=Cc1ccccc1
Mol. weight [g/mol]: 230.35
CAS: 20175-19-3

Physical Properties

Property code	Value	Unit	Source
gf	168.40	kJ/mol	Joback Method
hf	-115.19	kJ/mol	Joback Method
hfus	32.42	kJ/mol	Joback Method
hvap	60.24	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.629		Crippen Method
mcvol	209.810	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
ripol	2409.00		NIST Webbook
ripol	2409.00		NIST Webbook
tb	644.86	K	Joback Method
tc	847.89	K	Joback Method
tf	319.46	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.73	J/mol×K	644.86	Joback Method
cpg	566.77	J/mol×K	678.70	Joback Method
cpg	582.80	J/mol×K	712.54	Joback Method
cpg	597.87	J/mol×K	746.38	Joback Method
cpg	612.04	J/mol×K	780.22	Joback Method

cpg	625.36	J/mol×K	814.06	Joback Method
cpg	637.91	J/mol×K	847.89	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=C20175193&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume