Cinnamyl heptanoate

Inchi: InChI=1S/C16H22O2/c1-2-3-4-8-13-16(17)18-14-9-12-15-10-6-5-7-11-15/h5-7,9-12H,2-4
InchiKey: HVSYFKKRNSYXHZ-FMIVXFBMSA-N
Formula: C16H22O2
SMILES: CCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	42.55	kJ/mol	Joback Method
hf	-264.62	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	62.60	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.213		Crippen Method
mcvol	215.680	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	1909.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1905.00		NIST Webbook
ripol	2545.00		NIST Webbook
ripol	2545.00		NIST Webbook
tb	672.61	K	Joback Method
tc	874.88	K	Joback Method
tf	363.58	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.02	J/mol×K	672.61	Joback Method
cpg	594.72	J/mol×K	706.32	Joback Method
cpg	610.42	J/mol×K	740.03	Joback Method
cpg	625.19	J/mol×K	773.75	Joback Method

cpg	639.06	J/mol×K	807.46	Joback Method
cpg	652.07	J/mol×K	841.17	Joback Method
cpg	664.28	J/mol×K	874.88	Joback Method
dvisc	0.0016796	Pa×s	363.58	Joback Method
dvisc	0.0007941	Pa×s	415.09	Joback Method
dvisc	0.0004430	Pa×s	466.59	Joback Method
dvisc	0.0002775	Pa×s	518.10	Joback Method
dvisc	0.0001892	Pa×s	569.60	Joback Method
dvisc	0.0001374	Pa×s	621.11	Joback Method
dvisc	0.0001049	Pa×s	672.61	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=R201135&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
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
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