

2-Ethylhexyl trans-4-methoxycinnamate

Inchi:	InChI=1S/C18H26O3/c1-4-6-7-15(5-2)14-21-18(19)13-10-16-8-11-17(20-3)12-9-16/h8-13
InchiKey:	YBGZDTIWKVFCR-JLHYYAGUSA-N
Formula:	C18H26O3
SMILES:	CCCCC(CC)COC(=O)C=Cc1ccc(OC)cc1
Mol. weight [g/mol]:	290.40
CAS:	83834-59-7

Physical Properties

Property code	Value	Unit	Source
gf	-57.68	kJ/mol	Joback Method
hf	-454.87	kJ/mol	Joback Method
hfus	36.68	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.468		Crippen Method
mcvol	249.730	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2339.00		NIST Webbook
ripol	3122.00		NIST Webbook
tb	745.33	K	Joback Method
tc	946.17	K	Joback Method
tf	405.87	K	Joback Method
vc	0.952	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.03	J/molxK	745.33	Joback Method
cpg	734.08	J/molxK	778.80	Joback Method
cpg	750.11	J/molxK	812.28	Joback Method
cpg	765.14	J/molxK	845.75	Joback Method
cpg	779.20	J/molxK	879.22	Joback Method
cpg	792.33	J/molxK	912.69	Joback Method
cpg	804.55	J/molxK	946.17	Joback Method

dvisc	0.0009624	Paxs	405.87	Joback Method
dvisc	0.0004541	Paxs	462.45	Joback Method
dvisc	0.0002524	Paxs	519.02	Joback Method
dvisc	0.0001574	Paxs	575.60	Joback Method
dvisc	0.0001069	Paxs	632.18	Joback Method
dvisc	0.0000773	Paxs	688.75	Joback Method
dvisc	0.0000587	Paxs	745.33	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=C83834597&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
mvol:	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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