2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester

Other names: Octinoxate
Parsol MCX
Parsol MOX
2-Ethylhexyl p-methoxycinnamate
2-Ethylhexyl-4-methoxycinnamate
2-Ethylhexyl methoxycinnamate
3-(4-Methoxyphenyl)-2-propenoic acid 2-ethylhexyl ester
Escalol 557
Neo heliopan AV
Neo heliopan, type AV
Octyl methoxy cinnamate
2-Ethylhexyl 3-(4-methoxyphenyl)-2-propenoate
NSC 26466
Sunscreen AV
Uvinul MC 80
UvinulT MC 80 N

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: YBGZDTIWKVFICR-JLHYYAGUSA-N

Formula: C18H26O3

SMILES: CCCCC(CC)COC(=O)C=Cc1ccc(OC)cc1

Mol. weight [g/mol]: 290.40

CAS: 5466-77-3

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
tb	745.33	K	Joback Method
tc	946.17	K	Joback Method
tf	405.87	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.03	J/mol×K	745.33	Joback Method
cpg	734.08	J/mol×K	778.80	Joback Method
cpg	750.11	J/mol×K	812.28	Joback Method
cpg	765.14	J/mol×K	845.75	Joback Method
cpg	779.20	J/mol×K	879.22	Joback Method
cpg	792.33	J/mol×K	912.69	Joback Method
cpg	804.55	J/mol×K	946.17	Joback Method
dvisc	0.0009624	Pa×s	405.87	Joback Method
dvisc	0.0004541	Pa×s	462.45	Joback Method
dvisc	0.0002524	Pa×s	519.02	Joback Method
dvisc	0.0001574	Pa×s	575.60	Joback Method
dvisc	0.0001069	Pa×s	632.18	Joback Method
dvisc	0.0000773	Pa×s	688.75	Joback Method
dvisc	0.0000587	Pa×s	745.33	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=C5466773&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume