

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: YBGZDTIWKVFCR-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	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:	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=C5466773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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

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