2-ETHYLHEXYL P-(DIMETHYLAMINO)BENZOATE

Other names: 2-Ethylhexyl 4-dimethylaminobenzoate
p-Dimethylaminobenzoic acid 2-ethylhexyl ester
Benzoic acid, 4-(dimethylamino)-, 2-ethylhexyl ester
2-Ethylhexyl p-(dimethylamino)benzoate
Arlatone UVB
Escalol 507
4-(Dimethylamino)benzoic acid 2-ethylhexyl ester
Eusolex 6007
Octyl dimethyl PABA

Inchi: InChI=1S/C17H27NO2/c1-5-7-8-14(6-2)13-20-17(19)15-9-11-16(12-10-15)18(3)4/h9-12,1

InchiKey: WYWZRNAHINYAEF-UHFFFAOYSA-N

Formula: C17H27NO2

SMILES: CCCCC(CC)COC(=O)c1ccc(N(C)C)cc1

Mol. weight [g/mol]: 277.41

Physical Properties

Property code	Value	Unit	Source
af	0.7935		Cheméo Relay (1.0)
hfus	35.72	kJ/mol	Joback Method
log10ws	-5.05		Cheméo Relay (1.0)
logp	4.126		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2198.00		NIST Webbook
tb	614.50	K	Cheméo Relay (1.0)
tc	810.03	K	Cheméo Relay (1.0)
tf	292.18	K	Cheméo Relay (1.0)
vc	0.884	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.76	J/mol×K	708.31	Joback Method
cpg	713.53	J/mol×K	740.90	Joback Method

cpg	730.26	J/mol×K	773.49	Joback Method
cpg	745.99	J/mol×K	806.09	Joback Method
cpg	760.77	J/mol×K	838.68	Joback Method
cpg	774.61	J/mol×K	871.27	Joback Method
cpg	787.57	J/mol×K	903.86	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21245023&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume