Chrysanthemumic acid 2,4-dimethylbenzyl ester

Other names: Dimethrin

Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, (2,4-dimethylphenyl)methyl ester

Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, 2,4-dimethylbenzyl ester

Dimetrin

ENT 21,170

2,4-Dimethylbenzyl chrysanthemumate

2,4-Dimethylbenzyl 2,2-dimethyl-3-(2-methylpropenyl) cyclopropanecarboxylate

2,4-Dimethylbenzyl ester of chrysanthemumic acid

2,4-Dimethylbenzylester kyseliny chrysanthemove

(2,4-Dimethylphenyl)methyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylate

ENT-21170

NSC 15731

Inchi: InChI=1S/C19H26O2/c1-12(2)9-16-17(19(16,5)6)18(20)21-11-15-8-7-13(3)10-14(15)4/h7

InchiKey: FHNKBSDJERHDHZ-UHFFFAOYSA-N

Formula: C19H26O2

SMILES: CC(C)=CC1C(C(=O)OCc2ccc(C)cc2C)C1(C)C

Mol. weight [g/mol]: 286.41

CAS: 70-38-2

Physical Properties

Property code	Value	Unit	Source
gf	79.84	kJ/mol	Joback Method
hf	-311.91	kJ/mol	Joback Method
hfus	33.89	kJ/mol	Joback Method
hvap	68.83	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.585		Crippen Method
mcvol	247.090	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
tb	748.73	K	Joback Method
tc	965.61	K	Joback Method
tf	441.83	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.70	J/mol×K	748.73	Joback Method
cpg	747.96	J/mol×K	784.88	Joback Method
cpg	766.47	J/mol×K	821.02	Joback Method
cpg	784.37	J/mol×K	857.17	Joback Method
cpg	801.81	J/mol×K	893.32	Joback Method
cpg	818.93	J/mol×K	929.47	Joback Method
cpg	835.89	J/mol×K	965.61	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C70382&Units=SI

Legend

cpg: Ideal gas heat capacity
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