

Benzeneacetic acid, 4-chloro-«alpha»-(1-methylethyl)-, cyano (3-phenoxyphenyl)methyl ester, (S-(R*,R*))-

Other names:

Asana
Asana XL

(S)-«alpha»-Cyano-3-phenoxybenzyl(S)-2-(4-chlorophenyl)-3-methylbutyrate

Esfenvalerate

Fenvalerate «alpha»

Fenvalerate A «alpha»

Halmark

OMS 3023

S 1844

S 5602 A «alpha»

Sumi-alfa

Sumi-«alpha»

Sumicidin A «alpha»

(S)-alpha-Cyano-3-phenoxybenzyl(S)-2-(4-chlorophenyl)isovalerate

Benzeneacetic acid, 4-chloro-«alpha»-(1-methylethyl)-,

(S)-cyano(3-phenoxyphenyl)methyl ester, («alpha»S)-

[S-(R*,R*)]-cyano(3-phenoxyphenyl)methyl

-4-chloro-2-(1-methylethyl)benzeneacetate

esfenvalerate;

(S)-alpha-cyano-3-phenoxybenzyl-(S)-2-(4-chlorophenyl)-3-methylbutyrate

Inchi: InChI=1S/C25H22ClNO3/c1-17(2)24(18-11-13-20(26)14-12-18)25(28)30-23(16-27)19-7-

InchiKey: NYPJDWWKZLNNGM-ZEQRLZLVSA-N

Formula: C25H22ClNO3

SMILES: CC(C)C(C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1)c1ccc(Cl)cc1

Mol. weight [g/mol]: 419.90

CAS: 66230-04-4

Physical Properties

Property code	Value	Unit	Source
gf	252.60	kJ/mol	Joback Method
hf	-116.40	kJ/mol	Joback Method
hfus	40.96	kJ/mol	Joback Method
hvap	104.66	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.680		Crippen Method
mcvol	318.760	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	2861.00		NIST Webbook
tb	1098.30	K	Joback Method
tc	1359.75	K	Joback Method

tf	620.11	K	Joback Method
vc	1.210	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.65	J/mol×K	1098.30	Joback Method
cpg	994.49	J/mol×K	1141.87	Joback Method
cpg	1001.88	J/mol×K	1185.45	Joback Method
cpg	1007.90	J/mol×K	1229.02	Joback Method
cpg	1012.66	J/mol×K	1272.60	Joback Method
cpg	1016.26	J/mol×K	1316.17	Joback Method
cpg	1018.78	J/mol×K	1359.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66230044&Units=SI
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

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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