

Amigdalin, TFA

Inchi:	InChI=1S/C34H20F21NO18/c35-28(36,37)21(57)65-8-12-14(70-23(59)30(41,42)43)15(7
InchiKey:	ZHGNHOOVYPHPNJ-NEHBFDAQSA-N
Formula:	C34H20F21NO18
SMILES:	N#CC(OC1OC(COC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2O
Mol. weight [g/mol]:	1129.48

Physical Properties

Property code	Value	Unit	Source
gf	-5625.04	kJ/mol	Joback Method
hf	-6824.64	kJ/mol	Joback Method
hfus	118.70	kJ/mol	Joback Method
hvap	153.73	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	4.684		Crippen Method
mvol	558.550	ml/mol	McGowan Method
pc	480.07	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	1702.21	K	Joback Method
tc	3088.36	K	Joback Method
tf	1162.24	K	Joback Method
vc	2.256	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1707.93	J/molxK	1702.21	Joback Method
cpg	1465.56	J/molxK	1933.24	Joback Method
cpg	1172.84	J/molxK	2164.26	Joback Method
cpg	848.48	J/molxK	2395.29	Joback Method
cpg	511.17	J/molxK	2626.31	Joback Method
cpg	179.62	J/molxK	2857.34	Joback Method
cpg	-127.49	J/molxK	3088.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R322024&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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