Pyrazoline (diazomethane adduct of amorpha-4,9,11-trien-12-carboxylic acid)

Inchi: InChI=1S/C16H22N2O2/c1-9-4-5-14-13(6-9)12(10(2)15(19)20)7-11-8-17-18-16(11,14)3/h

InchiKey: ZRWSDQORPVPEFS-WBNCRLLSSA-N

Formula: C16H22N2O2

SMILES: C=C(C(=O)O)C1CC2CN=NC2(C)C2CCC(C)=CC12

Mol. weight [g/mol]: 274.36

Physical Properties

Property code	Value	Unit	Source
gf	294.18	kJ/mol	Joback Method
hf	-108.39	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	86.37	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.460		Crippen Method
mcvol	218.220	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1875.00		NIST Webbook
tb	846.99	K	Joback Method
tc	1083.18	K	Joback Method
tf	577.39	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.26	J/mol×K	846.99	Joback Method
cpg	784.02	J/mol×K	886.35	Joback Method
cpg	801.99	J/mol×K	925.72	Joback Method
cpg	819.32	J/mol×K	965.08	Joback Method
cpg	836.20	J/mol×K	1004.45	Joback Method
cpg	852.80	J/mol×K	1043.81	Joback Method
cpg	869.31	J/mol×K	1083.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R503367&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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