PROPAFENONE-H2O, M(DESAMINO-DI-IIO-), AC

Inchi: InChI=1S/C22H22O6/c1-16(23)26-13-6-14-27-22-12-10-19(28-17(2)24)15-20(22)21(25)1

InchiKey: PPJPAFBMLKJYTF-MKMNVTDBSA-N

Formula: C22H22O6

SMILES: CC(=O)OCC=COc1ccc(OC(C)=O)cc1C(=O)CCc1ccccc1

Mol. weight [g/mol]: 382.41

Physical Properties

Property code	Value	Unit	Source
gf	-281.62	kJ/mol	Joback Method
hf	-664.47	kJ/mol	Joback Method
hfus	48.60	kJ/mol	Joback Method
hvap	97.87	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.883		Crippen Method
mcvol	291.340	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2950.00		NIST Webbook
rinpol	2950.00		NIST Webbook
tb	999.11	K	Joback Method
tc	1234.00	K	Joback Method
tf	626.98	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.91	J/mol×K	999.11	Joback Method
cpg	913.75	J/mol×K	1038.26	Joback Method
cpg	923.18	J/mol×K	1077.41	Joback Method
cpg	931.24	J/mol×K	1116.56	Joback Method
cpg	937.96	J/mol×K	1155.71	Joback Method
cpg	943.38	J/mol×K	1194.85	Joback Method
cpg	947.55	J/mol×K	1234.00	Joback Method
dvisc	0.0002067	Pa×s	626.98	Joback Method

dvisc	0.0001264	Pa×s	689.00	Joback Method
dvisc	0.0000838	Pa×s	751.02	Joback Method
dvisc	0.0000592	Pa×s	813.05	Joback Method
dvisc	0.0000439	Pa×s	875.07	Joback Method
dvisc	0.0000339	Pa×s	937.09	Joback Method
dvisc	0.0000270	Pa×s	999.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255360&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
dvisc:	Dynamic viscosity
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