Dl-4-(2-benzoyloxyethyl)-2-phenyl-delta^2-thiazoli

Other names: Dl-4-(2-benzoyloxyethyl)-2-phenyl-delta
Inchi: InChI=1S/C18H17NO2S/c20-18(15-9-5-2-6-10-15)21-12-11-16-13-22-17(19-16)14-7-3-1-
InchiKey: FNQNEBUSCQXHGX-UHFFFAOYSA-N
Formula: C18H17NO2S
SMILES: O=C(OCCC1CSC(c2ccccc2)=N1)c1ccccc1
Mol. weight [g/mol]: 311.40
CAS: 94004-88-3

Physical Properties

Property code	Value	Unit	Source
gf	305.10	kJ/mol	Joback Method
hf	36.43	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	82.60	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.796		Crippen Method
mcvol	235.570	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
tb	861.84	K	Joback Method
tc	1129.84	K	Joback Method
tf	596.79	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.88	J/mol×K	861.84	Joback Method
cpg	722.15	J/mol×K	906.51	Joback Method
cpg	735.61	J/mol×K	951.17	Joback Method
cpg	747.35	J/mol×K	995.84	Joback Method
cpg	757.45	J/mol×K	1040.51	Joback Method
cpg	766.00	J/mol×K	1085.18	Joback Method
cpg	773.07	J/mol×K	1129.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94004883&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume