

Quantacure BMS

Other names:	Methanone, [4-[(4-methylphenyl)thio]phenyl]phenyl-4-(4-Methylphenylthio)benzophenone Phenyl (p-tolylthio)phenyl ketone Kayacure BMS Quantacure BMS (4-Benzoyl-4-methyldiphenyl sulfide)
Inchi:	InChI=1S/C20H16OS/c1-15-7-11-18(12-8-15)22-19-13-9-17(10-14-19)20(21)16-5-3-2-4-
InchiKey:	DBHQYYNDKZDVTN-UHFFFAOYSA-N
Formula:	C20H16OS
SMILES:	<chem>Cc1ccc(Sc2ccc(C(=O)c3ccccc3)cc2)cc1</chem>
Mol. weight [g/mol]:	304.40
CAS:	83846-85-9

Physical Properties

Property code	Value	Unit	Source
gf	339.69	kJ/mol	Joback Method
hf	159.81	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	81.83	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.377		Crippen Method
mcvol	239.300	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	2791.00		NIST Webbook
rinpol	2791.00		NIST Webbook
tb	869.65	K	Joback Method
tc	1145.76	K	Joback Method
tf	503.79	K	Joback Method
vc	0.891	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.59	J/mol×K	869.65	Joback Method
cpg	682.88	J/mol×K	915.67	Joback Method

cpg	695.61	J/mol×K	961.69	Joback Method
cpg	706.90	J/mol×K	1007.71	Joback Method
cpg	716.88	J/mol×K	1053.73	Joback Method
cpg	725.67	J/mol×K	1099.74	Joback Method
cpg	733.41	J/mol×K	1145.76	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83846859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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