

Glutril

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C18H26N2O4S/c1-11-5-7-12(8-6-11)25(23,24)20-16(22)19-14-13-9-10-18(4,15-17)/s1

RMTYNAPTNBHJHI-UHFFFAOYSA-N

C18H26N2O4S

Cc1ccc(S(=O)(=O)NC(=O)NC2C3CCC(C)(C2O)C3(C)C)cc1

366.48

26944-48-9

Physical Properties

Property code	Value	Unit	Source
hfus	48.08	kJ/mol	Joback Method
log10ws	-3.36		Cheméo Relay (1.0)
logp	2.169		Crippen Method
mcvol	274.490	ml/mol	McGowan Method
tf	465.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.77380e+02
Coeff. B	2.56397e+00
Coeff. C	-2.25586e-03
Coeff. D	8.42260e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/109-480-8/Glutril.pdf>

Generated by Cheméo on 2026-10-28 14:43:44.385060159 +0000 UTC m=+63667.447961606.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.