

N-(2,4-dimethylphenyl)-3-oxobutanamide

Inchi:	InChI=1S/C12H15NO2/c1-8-4-5-11(9(2)6-8)13-12(15)7-10(3)14/h4-6H,7H2,1-3H3,(H,13,
InchiKey:	HGVIAKXYAZRSEG-UHFFFAOYSA-N
Formula:	C12H15NO2
SMILES:	CC(=O)CC(=O)Nc1ccc(C)cc1C
Mol. weight [g/mol]:	205.26
CAS:	97-36-9

Physical Properties

Property code	Value	Unit	Source
hf	-332.15	kJ/mol	Cheméo Relay (1.0)
hfus	28.40	kJ/mol	Joback Method
ie	7.92	eV	Cheméo Relay (1.0)
logp	2.221		Crippen Method
mcvol	169.300	ml/mol	McGowan Method
tb	585.45	K	Cheméo Relay (1.0)
tf	363.15	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	1.81000e-01
Coeff. B	9.66160e-01
Coeff. C	-5.37320e-04
Coeff. D	9.97200e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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