

1,1-bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C17H34O4/c1-13-10-16(8,9)12-17(11-13,20-18-14(2,3)4)21-19-15(5,6)7/h13H,14-16H2,17H3

NALFRYPTRXKZPN-UHFFFAOYSA-N

C17H34O4

CC1CC(C)(C)CC(OOC(C)(C)C)(OOC(C)(C)C)C1

302.45

6731-36-8

Physical Properties

Property code	Value	Unit	Source
hfus	11.09	kJ/mol	Joback Method
logp	5.022		Crippen Method
mcvol	263.010	ml/mol	McGowan Method
tb	549.97	K	Cheméo Relay (1.0)
tf	243.15	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	-1.13220e+02
Coeff. B	2.27068e+00
Coeff. C	-1.83600e-03
Coeff. D	6.64900e-07
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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