

1,1',1'',1'''-(1,2,3,4-butanetetrayl)tetrakis-

Inchi: InChI=1S/C28H26/c1-5-13-23(14-6-1)21-27(25-17-9-3-10-18-25)28(26-19-11-4-12-20-26

InchiKey: AOEDHVIDHZGXAP-UHFFFAOYSA-N

Formula: C₂₈H₂₆

SMILES: c1ccc(CC(c2ccccc2)C(Cc2ccccc2)c2ccccc2)cc1

Mol. weight [g/mol]: 362.51

CAS: 806-69-9

Physical Properties

Property code	Value	Unit	Source
gf	629.64	kJ/mol	Joback Method
hf	314.31	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	86.25	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.039		Crippen Method
mcvol	310.340	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
tb	945.88	K	Joback Method
tc	1211.98	K	Joback Method
tf	363.00 ± 4.00	K	NIST Webbook
tf	363.00 ± 4.00	K	NIST Webbook
tf	363.00 ± 4.00	K	NIST Webbook
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.82	J/mol×K	945.88	Joback Method
cpg	987.22	J/mol×K	990.23	Joback Method
cpg	1003.16	J/mol×K	1034.58	Joback Method
cpg	1017.84	J/mol×K	1078.93	Joback Method
cpg	1031.49	J/mol×K	1123.28	Joback Method
cpg	1044.34	J/mol×K	1167.63	Joback Method
cpg	1056.60	J/mol×K	1211.98	Joback Method

dvisc	0.0007746	Pa×s	481.00	Joback Method
dvisc	0.0003117	Pa×s	558.48	Joback Method
dvisc	0.0001566	Pa×s	635.96	Joback Method
dvisc	0.0000913	Pa×s	713.44	Joback Method
dvisc	0.0000592	Pa×s	790.92	Joback Method
dvisc	0.0000415	Pa×s	868.40	Joback Method
dvisc	0.0000308	Pa×s	945.88	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C806699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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