

DEFEROXAMINE

Other names:	Butanediamide, N'-[5-[[4-[[5-(acetylhydroxyamino)pentyl]amino]-1,4-dioxobutyl]hydroxyamino]pentyl]-N-(5-aminopentyl)pentanamide Ba-33112 Deferoxamide B Deferoxamin Deferoxamine B Deferoxaminum Deferrioxamine Deferrioxamine B Desferan Desferex Desferin Desferral Desferrin Desferrioxamine Desferrioxamine B Df B DFOA DFOM Ferrioxamine B, N-benzoyl- N-Benzoylferrioxamine B Propionohydroxamic acid, N-(5-(3-((5-aminopentyl)hydroxycarbamoyl)propionamido)pentyl)-3-((5-(N-hydroxyacetamido)pentyl)hydroxycarbamoyl)-3,9,14,20,25-pentaazatriacontane-2,10,13,21,24-pentone, 30-amino-3,14,25-trihydroxy-3,9,14,20,25-pentaazatriacontane-2,10,13,21,24-pentaone NSC-527604 N-(5-(3-((5-Aminopentyl)hydroxycarbamoyl)propionamido)pentyl)-3-((5-(N-hydroxyacetamido)pentyl)hydroxycarbamoyl)-3,9,14,20,25-pentaazatriacontane-2,10,13,21,24-pentone Desferoxamine B N'-[5-[[4-[[5-(acetylhydroxyamino)pentyl]amino]-1,4-dioxobutyl]hydroxyamino]pentyl]-N-(5-aminopentyl)pentanamide (deferroxamine) InChI=1S/C25H48N6O8/c1-21(32)29(37)18-9-3-6-16-27-22(33)12-14-25(36)31(39)20-10
Inchi:	
InchiKey:	UBQYURCVBFRUQT-UHFFFAOYSA-N
Formula:	C25H48N6O8
SMILES:	CC(=O)N(O)CCCCCNC(=O)CCC(=O)N(O)CCCCCNC(=O)CCC(=O)N(O)CCCCCN
Mol. weight [g/mol]:	560.69

Physical Properties

Property code	Value	Unit	Source
hfus	105.22	kJ/mol	Joback Method

logp	0.922		Crippen Method
mcvol	448.450	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1724.99	J/mol×K	1527.48	Joback Method
cpg	1773.10	J/mol×K	1679.68	Joback Method
cpg	1834.05	J/mol×K	1831.89	Joback Method
cpg	1916.63	J/mol×K	1984.09	Joback Method
cpg	2029.61	J/mol×K	2136.29	Joback Method
cpg	2181.76	J/mol×K	2288.50	Joback Method
cpg	2381.86	J/mol×K	2440.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70519&Units=SI
Joback Method:	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

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