Deferoxamine

Other names:

Butanediamide, N'-[5-[[4-[[5-(acetylhydroxyamino)pentyl]amino]-1,4-dioxobutyl]hydroxyamino]pentyl]-N-(5
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-hydroxyacetam
3,9,14,20,25-Pentaazatriacontane-2,10,13,21,24-pentone, 30-amino-3,14,25-trihydroxy-
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-hydroxyacetam
Desferioxamine B acid
N'-[5-[[4-[[5-(acetylhydroxyamino)pentyl]amino]-1,4-dioxobutyl]-hydroxyamino]pentyl]-N-(5
(deferoxamine)

Inchi: InChI=1S/C25H48N6O8/c1-21(32)29(37)18-9-3-6-16-27-22(33)12-14-25(36)31(39)20-10
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]: 560.68
CAS: 70-51-9

Physical Properties

Property code	Value	Unit	Source

gf	-317.87	kJ/mol	Joback Method
hf	-1235.60	kJ/mol	Joback Method
hfus	105.22	kJ/mol	Joback Method
hvap	184.65	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	0.922		Crippen Method
mcvol	448.450	ml/mol	McGowan Method
pc	1149.10	kPa	Joback Method
tb	1527.48	K	Joback Method
tc	2440.70	K	Joback Method
tf	1089.61	K	Joback Method
vc	1.675	m3/kmol	Joback 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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg: Ideal gas heat capacity
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