Danthron

Other names:	1,8-Dihydroxy-9,10-anthracenedione
	1,8-Dihydroxy-9,10-anthraquinone
	1,8-Dihydroxyanthrachinon
	1,8-Dihydroxyanthraquinone
	9,10-Anthracenedione, 1,8-dihydroxy-
	Altan
	Anthraquinone, 1,8-dihydroxy-
	Antrapurol
	Chrysazin
	Criasazin
	Danivac
	Dantron
	Dantrone
	Diaquone
	Dionone
	Dorbane
	Duolax
	Istin
	Istizin
	LTAN
	Laxanorm
	Laxanthreen
	Laxipur
	Laxipurin
	Modane
	NSC 38626
	NSC 646568
	Prugol
	Roydan
	USAF ND-59
	Zwitsalax
Inchi:	InChI=1S/C14H8O4/c15-9-5-1-3-7-11(9)14(18)12-8(13(7)17)4-2-6-10(12)16/h1-6,15-16H
InchiKey:	QBPFLULOKWLNNW-UHFFFAOYSA-N
Formula:	C14H8O4
SMILES:	O=C1c2cccc(O)c2C(=O)c2c(O)cccc21
Mol. weight [g/mol]:	240.21
CAS:	117-10-2

Physical Properties

Property code	Value	Unit	Source
gf	-201.30	kJ/mol	Joback Method
hf	-412.89	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hsub	110.00 ± 8.00	kJ/mol	NIST Webbook
hvap	87.21	kJ/mol	Joback Method
log10ws	-5.19		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.873		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	4931.51	kPa	Joback Method
tb	887.06	K	Joback Method
tc	1170.41	K	Joback Method
tf	711.00	K	Joback Method
tt	435.39	K	Solid Forms, Crystal Habits, and Solubility of Danthron
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.57	J/mol×K	1075.96	Joback Method
cpg	545.52	J/mol×K	1123.19	Joback Method
cpg	484.36	J/mol×K	887.06	Joback Method
cpg	496.32	J/mol×K	934.29	Joback Method
cpg	508.20	J/mol×K	981.51	Joback Method
cpg	520.20	J/mol×K	1028.74	Joback Method
cpg	559.27	J/mol×K	1170.41	Joback Method
hsubt	106.00 ± 8.00	kJ/mol	404.00	NIST Webbook
hsubt	123.00	kJ/mol	368.00	NIST Webbook

Sources

Solid Forms, Crystal Habits, and Solubility of Danthron:	https://www.doi.org/10.1021/acs.jced.5b00192
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117102&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tt:	Triple Point Temperature
vc:	Critical Volume