

Butanediamide, 2,3-dihydroxy-N,N'-di-2-propenyl-

Other names:	N,N'-diallyltartramide
Inchi:	InChI=1S/C10H16N2O4/c1-3-5-11-9(15)7(13)8(14)10(16)12-6-4-2/h3-4,7-8,13-14H,1-2,5
InchiKey:	ZRKLEAHGBNDKHM-UHFFFAOYSA-N
Formula:	C10H16N2O4
SMILES:	C=CCNC(=O)C(O)C(O)C(=O)NCC=C
Mol. weight [g/mol]:	228.25
CAS:	28843-34-7

Physical Properties

Property code	Value	Unit	Source
gf	-148.58	kJ/mol	Joback Method
hf	-432.11	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	95.46	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	-1.687		Crippen Method
mcvol	178.000	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	813.12	K	Joback Method
tc	1003.41	K	Joback Method
tf	495.76	K	Joback Method
vc	0.665	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.68	J/molxK	813.12	Joback Method
cpg	532.54	J/molxK	844.83	Joback Method
cpg	540.84	J/molxK	876.55	Joback Method
cpg	548.62	J/molxK	908.26	Joback Method
cpg	555.91	J/molxK	939.98	Joback Method
cpg	562.73	J/molxK	971.69	Joback Method
cpg	569.12	J/molxK	1003.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28843347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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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