

Glutaric anhydride, 3-styryl-

Inchi:	InChI=1S/C13H12O3/c14-12-8-11(9-13(15)16-12)7-6-10-4-2-1-3-5-10/h1-7,11H,8-9H2/b
InchiKey:	ALGDBELJTXJZRR-VOTSOKGWSA-N
Formula:	C13H12O3
SMILES:	O=C1CC(C=Cc2ccccc2)CC(=O)O1
Mol. weight [g/mol]:	216.23
CAS:	116595-07-4

Physical Properties

Property code	Value	Unit	Source
gf	-55.64	kJ/mol	Joback Method
hf	-310.98	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	60.20	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.180		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	709.82	K	Joback Method
tc	978.74	K	Joback Method
tf	428.00	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.38	J/molxK	709.82	Joback Method
cpg	475.11	J/molxK	754.64	Joback Method
cpg	491.24	J/molxK	799.46	Joback Method
cpg	505.77	J/molxK	844.28	Joback Method
cpg	518.70	J/molxK	889.10	Joback Method
cpg	530.02	J/molxK	933.92	Joback Method
cpg	539.72	J/molxK	978.74	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=C116595074&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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