Eptam

Other names:	Alirox
	Carbamic acid, dipropylthio-, S-ethyl ester
	Carbamothioic acid, N,N-dipropyl-, S-ethyl ester
	Carbamothioic acid, dipropyl-, S-ethyl ester
	Dipropylcarbamothioic acid S-ethyl ester
	EPTC
	EPTC (pesticide)
	EPTC (pesticide, MW 189)
	Eptam 6E
	Ethyl N,N-di-n-propylthiocarbamate
	Ethyl N,N-dipropylthiolcarbamate
	Ethyl di-n-propylthiolcarbamate
	FDA 1541
	Genep EPTC
	N,N-Dipropylthiocarbamic acid S-ethyl ester
	NSC 40486
	Niptan
	R-1608
	S-Aethyl-N,N-dipropylthiolcarbamat
	S-Ethyl Dipropylthiocarbamate
	S-Ethyl N,N-di-n-propylthiocarbamate
	S-Ethyl N,N-di-n-propylthiolcarbamate
	S-Ethyl N,N-dipropylthiocarbamate
	Stauffer R 1608
	Torbin
	Witox
Inchi:	InChI=1S/C9H19NOS/c1-4-7-10(8-5-2)9(11)12-6-3/h4-8H2,1-3H3
InchiKey:	GUVLYNGULCJVDO-UHFFFAOYSA-N
Formula:	C9H19NOS
SMILES:	CCCN(CCC)C(=O)SCC
Mol. weight [g/mol]:	189.32
CAS:	759-94-4

Physical Properties

Property code	Value	Unit	Source
gf	39.88	kJ/mol	Joback Method

hf	-232.27	kJ/mol	Joback Method
hfus	27.82	kJ/mol	Joback Method
hvap	51.23	kJ/mol	Joback Method
log10ws	-2.70		Aqueous Solubility Prediction Method
logp	2.981		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1357.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1360.00		NIST Webbook
tb	540.41	K	Joback Method
tc	731.25	K	Joback Method
tf	307.99	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.44	J/mol×K	540.41	Joback Method
cpg	402.10	J/mol×K	572.22	Joback Method
cpg	416.05	J/mol×K	604.02	Joback Method
cpg	429.30	J/mol×K	635.83	Joback Method
cpg	441.87	J/mol×K	667.64	Joback Method
cpg	453.78	J/mol×K	699.44	Joback Method
cpg	465.05	J/mol×K	731.25	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C759944&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume