Carbamic acid, methyl-, p-[2-(3-methylureido)ethyl]phenyl ester

Inchi: InChI=1S/C12H17N3O3/c1-13-11(16)15-8-7-9-3-5-10(6-4-9)18-12(17)14-2/h3-6H,7-8H2,

InchiKey: BMJMOPYXKZMWRE-UHFFFAOYSA-N

Formula: C12H17N3O3

SMILES: CNC(=O)NCCc1ccc(OC(=O)NC)cc1

Mol. weight [g/mol]: 251.28

CAS: 91646-87-6

Physical Properties

Property code	Value	Unit	Source
gf	58.27	kJ/mol	Joback Method
hf	-262.92	kJ/mol	Joback Method
hfus	40.17	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	0.876		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	786.29	K	Joback Method
tc	999.61	K	Joback Method
tf	544.01	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.58	J/mol×K	786.29	Joback Method
cpg	576.72	J/mol×K	821.84	Joback Method
cpg	587.93	J/mol×K	857.40	Joback Method
cpg	598.23	J/mol×K	892.95	Joback Method
cpg	607.66	J/mol×K	928.50	Joback Method
cpg	616.24	J/mol×K	964.05	Joback Method
cpg	623.98	J/mol×K	999.61	Joback Method

Sources

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=C91646876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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