3-(METHYLTHIO)PENTA-2,4-DIONE

Inchi: InChI=1S/C6H10O2S/c1-4(7)6(9-3)5(2)8/h6H,1-3H3
InchiKey: HTVGCUNUQZCFAN-UHFFFAOYSA-N
Formula: C6H10O2S
SMILES: CSC(C(C)=O)C(C)=O
Mol. weight [g/mol]: 146.21

Physical Properties

Property code	Value	Unit	Source
af	0.3798		Cheméo Relay (1.0)
hf	-372.64	kJ/mol	Cheméo Relay (1.0)
hfus	15.10	kJ/mol	Joback Method
hvap	52.58	kJ/mol	Cheméo Relay (1.0)
ie	8.28	eV	Cheméo Relay (1.0)
log10ws	-0.30		Cheméo Relay (1.0)
logp	0.896		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
ripol	1703.00		NIST Webbook
ripol	1703.00		NIST Webbook
tb	481.94	K	Cheméo Relay (1.0)
tc	678.21	K	Cheméo Relay (1.0)
tf	291.07	K	Cheméo Relay (1.0)
vc	0.376	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.65	J/mol×K	512.76	Joback Method
cpg	247.99	J/mol×K	548.70	Joback Method
cpg	257.80	J/mol×K	584.63	Joback Method
cpg	267.09	J/mol×K	620.57	Joback Method
cpg	275.85	J/mol×K	656.50	Joback Method
cpg	284.10	J/mol×K	692.44	Joback Method
cpg	291.83	J/mol×K	728.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32113681&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume