BUTANE, 3-METHYL-1-(METHYLSULFINYL)-

Inchi: InChI=1S/C6H14OS/c1-6(2)4-5-8(3)7/h6H,4-5H2,1-3H3
InchiKey: LPQJPBDMUNOHNN-UHFFFAOYSA-N
Formula: C6H14OS
SMILES: CC(C)CCS(C)=O
Mol. weight [g/mol]: 134.24

Physical Properties

Property code	Value	Unit	Source
af	0.3931		Cheméo Relay (1.0)
gf	-220.51	kJ/mol	Joback Method
hf	-258.08	kJ/mol	Cheméo Relay (1.0)
hfus	15.53	kJ/mol	Joback Method
hvap	69.65	kJ/mol	Cheméo Relay (1.0)
ie	8.55 ± 0.05	eV	NIST Webbook
logp	1.411		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	493.01	K	Cheméo Relay (1.0)
tc	691.48	K	Cheméo Relay (1.0)
tf	298.88	K	Cheméo Relay (1.0)
vc	0.419	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.93	J/mol×K	394.52	Joback Method
cpg	229.71	J/mol×K	424.43	Joback Method
cpg	241.07	J/mol×K	454.34	Joback Method
cpg	252.01	J/mol×K	484.25	Joback Method
cpg	262.54	J/mol×K	514.15	Joback Method
cpg	272.65	J/mol×K	544.06	Joback Method
cpg	282.36	J/mol×K	573.97	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C55860101&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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