Propyl isopentyl sulfide

Inchi: InChI=1S/C8H18S/c1-4-6-9-7-5-8(2)3/h8H,4-7H2,1-3H3
InchiKey: NZPWRMRDLFXMPA-UHFFFAOYSA-N
Formula: C8H18S
SMILES: CCCSCCC(C)C
Mol. weight [g/mol]: 146.30

Physical Properties

Property code	Value	Unit	Source
af	0.3625		Cheméo Relay (1.0)
gf	47.16	kJ/mol	Joback Method
hf	-181.64	kJ/mol	Cheméo Relay (1.0)
hfus	17.08	kJ/mol	Joback Method
hvap	49.71	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-3.80		Cheméo Relay (1.0)
logp	3.176		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
tb	447.65	K	Cheméo Relay (1.0)
tc	630.72	K	Cheméo Relay (1.0)
tf	179.97	K	Cheméo Relay (1.0)
vc	0.507	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.04	J/mol×K	450.78	Joback Method
cpg	301.31	J/mol×K	482.41	Joback Method
cpg	315.00	J/mol×K	514.05	Joback Method
cpg	328.11	J/mol×K	545.68	Joback Method

cpg	340.66	J/mol×K	577.31	Joback Method
cpg	352.65	J/mol×K	608.94	Joback Method
cpg	364.09	J/mol×K	640.58	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=R157667&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
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