(Z)-7,7,7-Trifluoro-1,5-heptadiene

Inchi: InChI=1S/C7H9F3/c1-2-3-4-5-6-7(8,9)10/h2,5-6H,1,3-4H2/b6-5-
InchiKey: LLFYOFVOPGHZLL-WAYWQWQTSA-N
Formula: C7H9F3
SMILES: C=CCCC=CC(F)(F)F
Mol. weight [g/mol]: 150.14
CAS: 85685-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-405.47	kJ/mol	Joback Method
hf	-542.24	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	26.72	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	3.071		Crippen Method
mcvol	106.200	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	354.98	K	Joback Method
tc	513.72	K	Joback Method
tf	166.00	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.60	J/mol×K	354.98	Joback Method
cpg	202.65	J/mol×K	381.44	Joback Method
cpg	213.10	J/mol×K	407.89	Joback Method
cpg	222.97	J/mol×K	434.35	Joback Method
cpg	232.31	J/mol×K	460.81	Joback Method
cpg	241.12	J/mol×K	487.27	Joback Method
cpg	249.43	J/mol×K	513.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85685241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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