(E)-3,4,4-Trimethylpent-2-ene

Inchi: InChI=1S/C8H16/c1-6-7(2)8(3,4)5/h6H,1-5H3/b7-6+
InchiKey: FZQMZRXKWHQJAG-VOTSOKGWSA-N
Formula: C8H16
SMILES: CC=C(C)C(C)(C)C
Mol. weight [g/mol]: 112.21

Physical Properties

Property code	Value	Unit	Source
gf	90.99	kJ/mol	Joback Method
hf	-109.77	kJ/mol	Joback Method
hfus	7.95	kJ/mol	Joback Method
hvap	32.14	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	747.00		NIST Webbook
rinpol	759.10		NIST Webbook
rinpol	759.10		NIST Webbook
rinpol	745.10		NIST Webbook
tb	383.25	K	Joback Method
tc	570.42	K	Joback Method
tf	163.30	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.11	J/mol×K	383.25	Joback Method
cpg	233.89	J/mol×K	414.44	Joback Method
cpg	247.86	J/mol×K	445.64	Joback Method
cpg	261.06	J/mol×K	476.83	Joback Method
cpg	273.52	J/mol×K	508.03	Joback Method
cpg	285.30	J/mol×K	539.22	Joback Method

cpg	296.41	J/mol×K	570.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R292963&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume