54059766-2,4-dimethylhexane

Other names: 54059766-2,4-Dimethylhexane
Inchi: InChI=1S/C8H17Cl/c1-5-8(4,9)6-7(2)3/h7H,5-6H2,1-4H3
InchiKey: SYKUKUWLGOVGGT-UHFFFAOYSA-N
Formula: C8H17Cl
SMILES: CCC(C)(Cl)CC(C)C
Mol. weight [g/mol]: 148.68

Physical Properties

Property code	Value	Unit	Source
af	0.3334		Cheméo Relay (1.0)
gf	4.95	kJ/mol	Joback Method
hf	-261.94	kJ/mol	Cheméo Relay (1.0)
hfus	9.74	kJ/mol	Joback Method
hvap	41.22	kJ/mol	Cheméo Relay (1.0)
ie	9.70	eV	Cheméo Relay (1.0)
log10ws	-4.23		Cheméo Relay (1.0)
logp	3.440		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
tb	413.01	K	Cheméo Relay (1.0)
tc	603.16	K	Cheméo Relay (1.0)
tf	189.88	K	Cheméo Relay (1.0)
vc	0.488	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.66	J/mol×K	416.20	Joback Method
cpg	341.66	J/mol×K	602.32	Joback Method
cpg	330.49	J/mol×K	571.30	Joback Method
cpg	318.69	J/mol×K	540.28	Joback Method
cpg	306.24	J/mol×K	509.26	Joback Method
cpg	293.11	J/mol×K	478.24	Joback Method
cpg	279.26	J/mol×K	447.22	Joback Method

dvisc	0.0010487	Pa×s	306.73	Joback Method
dvisc	0.0002864	Pa×s	416.20	Joback Method
dvisc	0.0004062	Pa×s	379.71	Joback Method
dvisc	0.0006206	Pa×s	343.22	Joback Method
dvisc	0.0162102	Pa×s	197.26	Joback Method
dvisc	0.0020416	Pa×s	270.24	Joback Method
dvisc	0.0048938	Pa×s	233.75	Joback Method

Sources

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=C54059766&Units=SI
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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume