Z,z-6,25-tetratriactontadien-2-one

Other names: (6Z,25Z)-6,25-Tetratriacontadien-2-one
Z,Z-6,25-Tetratriacontadien-2-one
Inchi: InChI=1S/C34H64O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: QHFMHIUBQJRJIF-YVZJDIIDSA-N
Formula: C34H64O
SMILES: CCCCCCCC/C=C\CCCCCCCCCCCCCCCCC/C=C\CCCC(C)=O
Mol. weight [g/mol]: 488.88

Physical Properties

Property code	Value	Unit	Source
af	1.2611		Cheméo Relay (1.0)
gf	266.92	kJ/mol	Joback Method
hf	-765.06	kJ/mol	Cheméo Relay (1.0)
hfus	85.82	kJ/mol	Joback Method
hvap	168.24	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
log10ws	-10.19		Cheméo Relay (1.0)
logp	12.240		Crippen Method
mcvol	482.890	ml/mol	McGowan Method
pc	537.08	kPa	Joback Method
tb	681.83	K	Cheméo Relay (1.0)
tc	886.22	K	Cheméo Relay (1.0)
tf	312.19	K	Cheméo Relay (1.0)
vc	1.802	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1729.47	J/mol×K	1039.51	Joback Method
cpg	1759.43	J/mol×K	1084.02	Joback Method
cpg	1787.75	J/mol×K	1128.53	Joback Method
cpg	1814.67	J/mol×K	1173.04	Joback Method
cpg	1840.45	J/mol×K	1217.54	Joback Method
cpg	1865.33	J/mol×K	1262.05	Joback Method

cpg	1889.59	J/mol×K	1306.56	Joback Method
dvisc	0.0003701	Pa×s	512.71	Joback Method
dvisc	0.0001285	Pa×s	600.51	Joback Method
dvisc	0.0000584	Pa×s	688.31	Joback Method
dvisc	0.0000317	Pa×s	776.11	Joback Method
dvisc	0.0000195	Pa×s	863.91	Joback Method
dvisc	0.0000131	Pa×s	951.71	Joback Method
dvisc	0.0000095	Pa×s	1039.51	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U111389&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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