1,21-DOCOSADIENE

Other names: docosa-1,21-diene
Inchi: InChI=1S/C22H42/c1-3-5-7-9-11-13-15-17-19-21-22-20-18-16-14-12-10-8-6-4-2/h3-4H,1-
InchiKey: RBJABTJRYMHYOP-UHFFFAOYSA-N
Formula: C22H42
SMILES: C=CCCCCCCCCCCCCCCCCCCCC=C
Mol. weight [g/mol]: 306.58

Physical Properties

Property code	Value	Unit	Source
af	0.8773		Cheméo Relay (1.0)
gf	310.04	kJ/mol	Joback Method
hf	-313.10	kJ/mol	Cheméo Relay (1.0)
hfus	50.18	kJ/mol	Joback Method
hvap	109.45	kJ/mol	Cheméo Relay (1.0)
ie	9.52	eV	Cheméo Relay (1.0)
log10ws	-8.51		Cheméo Relay (1.0)
logp	8.380		Crippen Method
mcvol	312.240	ml/mol	McGowan Method
pc	949.08	kPa	Joback Method
tb	618.11	K	Cheméo Relay (1.0)
tc	769.44	K	Cheméo Relay (1.0)
tf	303.40 ± 2.00	K	NIST Webbook
tf	304.00 ± 3.00	K	NIST Webbook
vc	1.212	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.26	J/mol×K	696.12	Joback Method
cpg	933.08	J/mol×K	723.69	Joback Method
cpg	952.98	J/mol×K	751.26	Joback Method
cpg	972.00	J/mol×K	778.83	Joback Method
cpg	990.19	J/mol×K	806.40	Joback Method
cpg	1007.58	J/mol×K	833.98	Joback Method

cpg	1024.19	J/mol×K	861.55	Joback Method
dvisc	0.0027872	Pa×s	334.18	Joback Method
dvisc	0.0009948	Pa×s	394.50	Joback Method
dvisc	0.0004666	Pa×s	454.83	Joback Method
dvisc	0.0002613	Pa×s	515.15	Joback Method
dvisc	0.0001653	Pa×s	575.47	Joback Method
dvisc	0.0001140	Pa×s	635.80	Joback Method
dvisc	0.0000839	Pa×s	696.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53057537&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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