docosane, 1-iodo-

Inchi: InChI=1S/C22H45I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23/h2-2
InchiKey: QQTWESGWRGHHPL-UHFFFAOYSA-N
Formula: C22H45I
SMILES: CCCCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]: 436.50
CAS: 62127-53-1

Physical Properties

Property code	Value	Unit	Source
af	0.9690		Cheméo Relay (1.0)
gf	192.48	kJ/mol	Joback Method
hf	-444.17	kJ/mol	Cheméo Relay (1.0)
hfus	57.14	kJ/mol	Joback Method
hvap	127.90	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-9.43		Cheméo Relay (1.0)
logp	9.243		Crippen Method
mcvol	346.660	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
tb	636.23	K	Cheméo Relay (1.0)
tc	822.81	K	Cheméo Relay (1.0)
tf	321.02	K	Cheméo Relay (1.0)
vc	1.361	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.95	J/mol×K	795.90	Joback Method
cpg	1064.48	J/mol×K	826.49	Joback Method
cpg	1084.01	J/mol×K	857.07	Joback Method
cpg	1102.59	J/mol×K	887.66	Joback Method
cpg	1120.27	J/mol×K	918.25	Joback Method
cpg	1137.11	J/mol×K	948.84	Joback Method
cpg	1153.14	J/mol×K	979.42	Joback Method

dvisc	0.0017848	Pa×s	395.76	Joback Method
dvisc	0.0006583	Pa×s	462.45	Joback Method
dvisc	0.0003122	Pa×s	529.14	Joback Method
dvisc	0.0001750	Pa×s	595.83	Joback Method
dvisc	0.0001102	Pa×s	662.52	Joback Method
dvisc	0.0000755	Pa×s	729.21	Joback Method
dvisc	0.0000551	Pa×s	795.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62127531&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

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