octacosane, 1-iodo-

Inchi: InChI=1S/C28H57I/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey: HTERHJSPVTYONY-UHFFFAOYSA-N
Formula: C28H57I
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]: 520.66
CAS: 62154-80-7

Physical Properties

Property code	Value	Unit	Source
af	1.1798		Cheméo Relay (1.0)
gf	243.00	kJ/mol	Joback Method
hf	-569.35	kJ/mol	Cheméo Relay (1.0)
hfus	72.68	kJ/mol	Joback Method
hvap	156.91	kJ/mol	Cheméo Relay (1.0)
ie	9.73	eV	Cheméo Relay (1.0)
log10ws	-11.07		Cheméo Relay (1.0)
logp	11.584		Crippen Method
mcvol	431.200	ml/mol	McGowan Method
pc	648.12	kPa	Joback Method
tb	673.29	K	Cheméo Relay (1.0)
tc	858.73	K	Cheméo Relay (1.0)
tf	333.44	K	Cheméo Relay (1.0)
vc	1.692	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1428.84	J/mol×K	933.18	Joback Method
cpg	1452.87	J/mol×K	968.62	Joback Method
cpg	1475.58	J/mol×K	1004.05	Joback Method
cpg	1497.05	J/mol×K	1039.49	Joback Method
cpg	1517.39	J/mol×K	1074.93	Joback Method
cpg	1536.69	J/mol×K	1110.36	Joback Method
cpg	1555.05	J/mol×K	1145.80	Joback Method

dvisc	0.0007957	Pa×s	463.38	Joback Method
dvisc	0.0002840	Pa×s	541.68	Joback Method
dvisc	0.0001315	Pa×s	619.98	Joback Method
dvisc	0.0000724	Pa×s	698.28	Joback Method
dvisc	0.0000449	Pa×s	776.58	Joback Method
dvisc	0.0000304	Pa×s	854.88	Joback Method
dvisc	0.0000220	Pa×s	933.18	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62154807&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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