(1E,3E,7E,11E)-4-Isopropyl-1,7,11-trimethylcyclote

Inchi: InChI=1S/C20H32/c1-16(2)20-14-12-18(4)10-6-8-17(3)9-7-11-19(5)13-15-20/h8,11-12,14
InchiKey: UJUWZMUCEGGBOH-YBJPMODXSA-N
Formula: C20H32
SMILES: CC1=CC=C(C(C)C)CCC(C)=CCCC(C)=CCC1
Mol. weight [g/mol]: 272.47
CAS: 64363-64-0

Physical Properties

Property code	Value	Unit	Source
gf	131.76	kJ/mol	Joback Method
hf	-250.79	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	65.66	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.762		Crippen Method
mcvol	264.600	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2019.50		NIST Webbook
tb	731.50	K	Joback Method
tc	966.97	K	Joback Method
tf	336.74	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.95	J/mol×K	731.50	Joback Method
cpg	798.46	J/mol×K	770.74	Joback Method
cpg	821.98	J/mol×K	809.99	Joback Method
cpg	843.49	J/mol×K	849.23	Joback Method
cpg	862.95	J/mol×K	888.48	Joback Method
cpg	880.36	J/mol×K	927.72	Joback Method
cpg	895.69	J/mol×K	966.97	Joback Method
dvisc	0.0027490	Pa×s	336.74	Joback Method

dvisc	0.0004514	Pa×s	402.53	Joback Method
dvisc	0.0001231	Pa×s	468.33	Joback Method
dvisc	0.0000463	Pa×s	534.12	Joback Method
dvisc	0.0000215	Pa×s	599.91	Joback Method
dvisc	0.0000117	Pa×s	665.71	Joback Method
dvisc	0.0000071	Pa×s	731.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64363640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume