

Cyclopropaneoctanoic acid, 2-[[2-[(2-ethylcyclopropyl)methyl]cyclopropyl]methyl ester

Inchi: InChI=1S/C22H38O2/c1-3-16-11-18(16)13-20-15-21(20)14-19-12-17(19)9-7-5-4-6-8-10-2
InchiKey: KDWSWRXUIMELKF-UHFFFAOYSA-N

Formula: C22H38O2
SMILES: CCC1CC1CC1CC1CC1CC1CCCCCCCC(=O)OC
Mol. weight [g/mol]: 334.54
CAS: 10152-71-3

Physical Properties

Property code	Value	Unit	Source
gf	59.56	kJ/mol	Joback Method
hf	-584.83	kJ/mol	Joback Method
hfus	53.14	kJ/mol	Joback Method
hvap	72.53	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.989		Crippen Method
mcvol	295.700	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
rinpol	2350.00		NIST Webbook
tb	785.26	K	Joback Method
tc	975.12	K	Joback Method
tf	450.96	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.01	J/molxK	785.26	Joback Method
cpg	1015.61	J/molxK	816.90	Joback Method
cpg	1036.09	J/molxK	848.55	Joback Method
cpg	1055.53	J/molxK	880.19	Joback Method
cpg	1074.01	J/molxK	911.84	Joback Method
cpg	1091.59	J/molxK	943.48	Joback Method
cpg	1108.37	J/molxK	975.12	Joback Method
dvisc	0.0044185	Paxs	450.96	Joback Method

dvisc	0.0039500	Paxs	506.68	Joback Method
dvisc	0.0036105	Paxs	562.39	Joback Method
dvisc	0.0033540	Paxs	618.11	Joback Method
dvisc	0.0031540	Paxs	673.83	Joback Method
dvisc	0.0029939	Paxs	729.54	Joback Method
dvisc	0.0028630	Paxs	785.26	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10152713&Units=SI

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

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