

6-Methoxyeugenyl isovalerate

Inchi:	InChI=1S/C16H22O4/c1-6-7-12-9-13(18-4)16(14(10-12)19-5)20-15(17)8-11(2)3/h6,9-11H
InchiKey:	JWXZLHSHKHNEXMZ-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	C=CCc1cc(OC)c(OC(=O)CC(C)C)c(OC)c1
Mol. weight [g/mol]:	278.34
CAS:	957467-00-4

Physical Properties

Property code	Value	Unit	Source
gf	-191.16	kJ/mol	Joback Method
hf	-560.54	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	68.39	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.384		Crippen Method
mvol	227.420	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	1951.40		NIST Webbook
rinpol	1951.40		NIST Webbook
tb	724.47	K	Joback Method
tc	926.05	K	Joback Method
tf	433.92	K	Joback Method
vc	0.859	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.83	J/molxK	724.47	Joback Method
cpg	647.64	J/molxK	758.07	Joback Method
cpg	662.52	J/molxK	791.66	Joback Method
cpg	676.46	J/molxK	825.26	Joback Method
cpg	689.47	J/molxK	858.86	Joback Method
cpg	701.52	J/molxK	892.45	Joback Method
cpg	712.63	J/molxK	926.05	Joback Method

dvisc	0.0005834	Paxs	433.92	Joback Method
dvisc	0.0003441	Paxs	482.35	Joback Method
dvisc	0.0002235	Paxs	530.77	Joback Method
dvisc	0.0001560	Paxs	579.19	Joback Method
dvisc	0.0001151	Paxs	627.62	Joback Method
dvisc	0.0000887	Paxs	676.04	Joback Method
dvisc	0.0000708	Paxs	724.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C957467004&Units=SI
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

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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