

Bicyclo[2,2,1]hept-5-ene-2,3-dicarboxylic acid, bis(2-ethylhexyl)ester

Inchi:	InChI=1S/C25H42O4/c1-5-9-11-18(7-3)16-28-24(26)22-20-13-14-21(15-20)23(22)25(27)
InchiKey:	GUVQPBGSPLOPRC-UHFFFAOYSA-N
Formula:	C25H42O4
SMILES:	CCCCC(CC)COC(=O)C1C2C=CC(C2)C1C(=O)OCC(CC)CCCC
Mol. weight [g/mol]:	406.60
CAS:	47616-64-8

Physical Properties

Property code	Value	Unit	Source
gf	-189.16	kJ/mol	Joback Method
hf	-902.95	kJ/mol	Joback Method
hfus	56.57	kJ/mol	Joback Method
hvap	88.45	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.944		Crippen Method
mcvol	351.970	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
tb	930.67	K	Joback Method
tc	1139.93	K	Joback Method
tf	510.47	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.73	J/molxK	930.67	Joback Method
cpg	1316.15	J/molxK	1105.05	Joback Method
cpg	1301.51	J/molxK	1070.18	Joback Method
cpg	1285.72	J/molxK	1035.30	Joback Method
cpg	1268.70	J/molxK	1000.42	Joback Method
cpg	1250.40	J/molxK	965.55	Joback Method
cpg	1329.71	J/molxK	1139.93	Joback Method
dvisc	0.0002931	Paxs	930.67	Joback Method
dvisc	0.0003512	Paxs	860.64	Joback Method

dvisc	0.0004344	Paxs	790.60	Joback Method
dvisc	0.0005601	Paxs	720.57	Joback Method
dvisc	0.0007628	Paxs	650.54	Joback Method
dvisc	0.0011192	Paxs	580.50	Joback Method
dvisc	0.0018243	Paxs	510.47	Joback Method

Sources

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=C47616648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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