2-Ethoxyethyl 3,5,5-trimethylhexanoate

Inchi: InChI=1S/C13H26O3/c1-6-15-7-8-16-12(14)9-11(2)10-13(3,4)5/h11H,6-10H2,1-5H3
InchiKey: HJZJPDVJUZKWJK-UHFFFAOYSA-N
Formula: C13H26O3
SMILES: CCOCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 230.34

Physical Properties

Property code	Value	Unit	Source
gf	-279.94	kJ/mol	Joback Method
hf	-702.70	kJ/mol	Joback Method
hfus	22.46	kJ/mol	Joback Method
hvap	54.41	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	3.029		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	1422.00		NIST Webbook
rinpol	1422.00		NIST Webbook
tb	591.88	K	Joback Method
tc	771.51	K	Joback Method
tf	318.08	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.68	J/mol×K	591.88	Joback Method
cpg	563.84	J/mol×K	621.82	Joback Method
cpg	580.20	J/mol×K	651.76	Joback Method
cpg	595.80	J/mol×K	681.70	Joback Method
cpg	610.64	J/mol×K	711.64	Joback Method
cpg	624.74	J/mol×K	741.58	Joback Method
cpg	638.12	J/mol×K	771.51	Joback Method
dvisc	0.0032170	Pa×s	318.08	Joback Method

dvisc	0.0012969	Pa×s	363.71	Joback Method
dvisc	0.0006402	Pa×s	409.35	Joback Method
dvisc	0.0003641	Pa×s	454.98	Joback Method
dvisc	0.0002295	Pa×s	500.61	Joback Method
dvisc	0.0001563	Pa×s	546.25	Joback Method
dvisc	0.0001129	Pa×s	591.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378271&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