di-n-Amylfumarate

Other names: Dipentyl fumarate
Inchi: InChI=1S/C14H24O4/c1-3-5-7-11-17-13(15)9-10-14(16)18-12-8-6-4-2/h9-10H,3-8,11-12H
InchiKey: NFCMRHDORQSGIS-MDZDMXLPSA-N
Formula: C14H24O4
SMILES: CCCCCOC(=O)C=CC(=O)OCCCCC
Mol. weight [g/mol]: 256.34
CAS: 20314-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-320.62	kJ/mol	Joback Method
hf	-704.67	kJ/mol	Joback Method
hfus	37.79	kJ/mol	Joback Method
hvap	65.03	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.009		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1558.00		NIST Webbook
tb	676.46	K	Joback Method
tc	857.71	K	Joback Method
tf	386.78	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.12	J/mol×K	676.46	Joback Method
cpg	668.66	J/mol×K	827.50	Joback Method
cpg	656.37	J/mol×K	797.29	Joback Method
cpg	643.39	J/mol×K	767.08	Joback Method
cpg	629.69	J/mol×K	736.88	Joback Method
cpg	615.28	J/mol×K	706.67	Joback Method
cpg	680.26	J/mol×K	857.71	Joback Method

dvisc	0.0001031	Pa×s	676.46	Joback Method
dvisc	0.0001345	Pa×s	628.18	Joback Method
dvisc	0.0001834	Pa×s	579.90	Joback Method
dvisc	0.0002647	Pa×s	531.62	Joback Method
dvisc	0.0004109	Pa×s	483.34	Joback Method
dvisc	0.0007034	Pa×s	435.06	Joback Method
dvisc	0.0013772	Pa×s	386.78	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	465.00 ± 1.00	K	3.30	NIST Webbook

Sources

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=C20314743&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume